Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

February 10, 2017

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System Maintenance Activities Completed During Dedicated Time

- System engineers successfully completed maintenance activities on the HECC systems and recovered from a power event during the scheduled maintenance downtime on Feb. 6–7.
- Activities completed include:
  - Applied operating system patches and software updates.
  - Updated InfiniBand firmware on switches and nodes.
  - Replaced faulty hardware components.
  - Updated nobackupp1 Lustre servers with new caching subsystem and storage.
  - Tested and debugged InfiniBand fabric.
  - Updated the PBS batch scheduler software.
- Just as the systems were being returned to the production phase of the downtime, a power event occurred at Ames, resulting in the loss of power to all HECC systems. System engineers were able to bring the majority of systems up within the day.
- The archive system recovery took two weeks due to issues with the filesystems, which were brought back online intact without any data loss.

Mission Impact: Regular maintenance on the HECC systems provides a stable and well-performing computing environment for NASA users.

HECC systems were in a 24-hour dedicated time for system maintenance activities in early February.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing (NAS) Division;
Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NAS Division, CSRA LLC

Facilities Team Reconfigures RUPS to Protect Additional HECC Resources

- On February 22, the Rotary Uninterruptible Power Supply (RUPS) was reconfigured from a 1+1 (1 active and 1 stand-by unit) to a 2+0 (2 active and 0 stand-by units) to provide UPS protection for HECC filesystems and the main communications room in the main NAS facility, building N258.
- The facility now has approximately 3.3 megawatts (MW) of load on the RUPS with a 4 MW capacity.
- The HECC Facilities team worked with Ames engineering to obtain authorization to put the RUPS in the N configuration, allowing additional resources to be protected.
- This new configuration improves the HECC project's ability to protect user data and network from future building power failures.
- Now, when N258 has a power outage the RUPS protects all user data, and remote access to HECC resources is retained.

Mission Impact: Protecting scientific data is crucial to NASA users, and maintaining network access during power outages is critical to returning HECC resources to full operation with minimal impact.

The rotary uninterruptible power supply units behind the main supercomputing facility (building N258) at Ames Research Center. A new configuration now protects HECC filesystems and the main N258 communications room.

POCs: William Thigpen, william.w.thigpen@nasa.gov, (650) 604-1061, NASA Advanced Supercomputing (NAS) Division;
Chris Tanner, christopher.tanner@nasa.gov, (650) 604-6754, NAS Division, CSRA LLC

User Services Team Completes Replacement of RSA SecurID Tokens

- A more efficient procedure was developed for replacing expiring RSA SecurID tokens allowing users to select either physical or logical tokens online.
- The HECC User Services team replaced approximately 548 out of 633 electronic tokens that expired on February 28, 2017.
- During the process, all active NAS accounts linked to expiring tokens were reviewed for accuracy.
- Once the analysis was complete, HECC users were invited to select either a replacement software token or a physical token fob using a new web-based interface created for this purpose.
- 188 new soft tokens were distributed, and 360 token fobs were either mailed or prepared for pickup by onsite users. Another 85 users did not respond to multiple notifications that were sent.
- User Services staff worked directly with Two-Factor Token Infrastructure (TFTI) administrators to bulk-load replacement token fobs and streamline the activation process.

Mission Impact: RSA SecurID tokens are the foundation of authenticating to the HECC environment, providing continuous and secure access to resources and data.

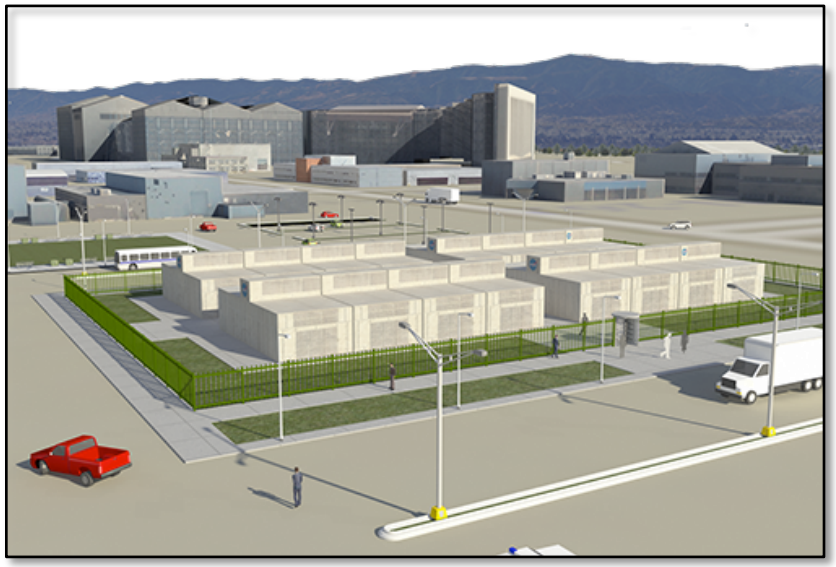
Sample inventory of new token fobs that were purchased to replace tokens expiring on February 28, 2017.

POC: Leigh Ann Tanner, leighann.tanner@nasa.gov, (650) 604-4468, NASA Advanced Supercomputing Division, CSRA LCC

NAS Facility Expansion Team Issues RFI, Hosts Industry Day and Vendor Briefings

- The NAS Facility Expansion (NFE) team released a Request for Information and received responses from 8 vendors who showed a high level of interest in the project and the ability to meet its requirements.
- On February 21, NASA and staff from CSRA, the government contractor conducting the procurement, held an "industry day" for the vendors. The agenda included a briefing and tours of the proposed site, the Modular Supercomputer Facility, and the main NAS facility, building N258.
- Subsequently, vendors gave one-on-one briefings to the NFE team, outlining how they would be able to respond to a Request for Proposal (RFP).
- The NFE procurement team is in the process of writing the RFP, and intends to release a draft in March and the final version in May. They expect to make a selection in the summer and award a contract in October 2017.

Mission Impact: Expanding its ability to host new computer hardware is a key part of the HECC Project's strategy of providing NASA mission directorates with sufficient state-of-the-art resources to meet their computing capacity and capability requirements.



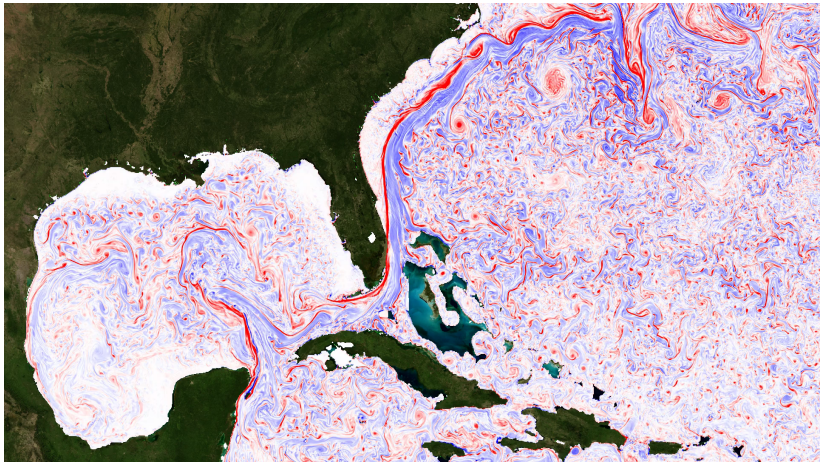
Artist's concept of what the NAS facility expansion might look like on completion in 2022. Existing buildings at NASA Ames are shown in the background. *Marco Librero, NASA/Ames*

POCs: Robert Hood, robert.hood@nasa.gov, NASA Advanced Supercomputing (NAS) Division, CSRA LLC.

Simulating Global Ocean Circulation Across 70,000 Pleiades Cores

- Researchers from the Estimating the Circulation and Climate of the Ocean (ECCO) consortium are running simulations on Pleiades to produce global, time-evolving maps of Earth's ocean and sea-ice system at an unprecedented resolution—about 1 kilometer (km) horizontal grid spacing.
- The simulations are produced with the Massachusetts Institute of Technology general circulation model (MITgcm) across up to 70,000 Pleiades cores. They are used to:
  - Investigate fundamental questions such as how the circulation, chemistry, and biology of the ocean collectively interact with atmospheric carbon.
  - Explore where and when heat is absorbed by or released from the ocean.
  - Determine how a pollutant plume or debris field might spread from a particular ocean location.
  - Design in-situ observing systems, and satellite missions to better monitor and understand ocean turbulence and its impacts on Earth's critical, life-supporting climate systems.
- Next steps include coupling the model with an interactive atmospheric model of similar resolution.

Mission Impact: Enabled by HECC resources, this work will help design NASA missions such as the Surface Water and Ocean Topography, and will aid researchers in understanding and potentially predicting the impact of global ocean circulation on climate.



This movie of a high-resolution MITgcm simulation reveals new details of the ocean's surface vorticity, providing researchers a never-before-seen look at the tremendous complexity of ocean variability, including surface signatures of geostrophic eddies, sub-mesoscale eddies, and internal tides. *Christopher Henze, NASA/Ames*

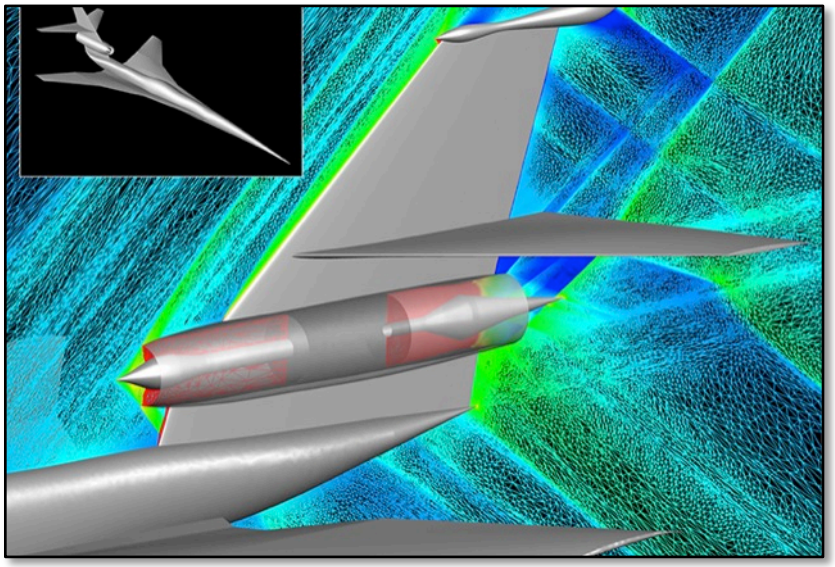
POCs: Christopher Hill, cnh@mit.edu, (617) 253-6430, Massachusetts Institute of Technology;
Dimitris Menemenlis, dimitris.menemenlis@jpl.nasa.gov, (818) 354-1656, NASA JPL

FUN3D Solver Optimized for Unstructured Grid Applications on Pleiades GPUs *

- To efficiently leverage next-generation systems consisting of heterogeneous CPU/GPU combinations, researchers at Old Dominion University, NASA Langley, and NVIDIA Corporation implemented extensive optimization of the FUN3D linear solver using the GPU nodes on Pleiades.
  - Results were generated on Pleiades using an Intel Xeon E5-2670 dual socket, eight-core processor with an NVIDIA Tesla K40 GPU accelerator.
  - The team developed alternative implementations of existing CUDA library functions appropriate for sparse matrix-vector products and triangular solutions of matrices typically encountered in FUN3D simulations.
- The new implementation shows performance gains of up to seven times that of the approach based on existing CUDA library functions for a broad range of matrix and block sizes.
- Work was presented in a paper for the SC16 Workshop on Irregular Applications: Architectures and Algorithms.
- Follow-on work has resulted in substantially increased speedups using an improved data layout and newer NVIDIA Pascal hardware.

** HECC provided supercomputing resources and services in support of this work.*

Mission Impact: Performing extensive optimization of the FUN3D sparse-matrix linear solver kernel on the NVIDIA K40 GPU nodes of HECC's Pleiades supercomputer demonstrates that computationally intensive flowfield calculations can be efficiently performed using such hardware.



Adjoint-based adaptation for a supersonic internal/external flow over a low-boom demonstrator aircraft configuration. The mesh is colored by pressure magnitude; red indicates high values, blue indicates low values. *Chris Heath, NASA Glenn*

POCs: Mohammad Zubair, zubair@cs.odu.edu, (757) 683-3917, Old Dominion University; Eric Nielsen, eric.j.nielsen@nasa.gov, (757) 864-2239, NASA Langley Research Center

HECC Facility Hosts Several Visitors and Tours in February 2017

- HECC hosted 13 tour groups in February; guests learned about the agency-wide missions being supported by HECC assets, and some groups also viewed the D-Wave 2X quantum computer system. Visitors this month included:
  - Pierre Franck, Luxembourg Consul General.
  - Chris Culbert, Chief Technologist at JSC.
  - Barbara Block, Professor of Biological Sciences at Stanford University.
  - Rosie Rios, who served as the 43rd Treasurer of the United States.
  - Rick Davis, Assistant Director for Science and Exploration in the Planetary Science Division at NASA HQ.
  - A large group from the Ames Early Career Network.
  - 12 international students from the Tokyo University of Science.
  - 20 students (juniors and seniors) and instructors from Red Bluff High School, who are participating in NASA's Lassen Astrobiology Intern Program.

NAS Division Computational Aerosciences Branch Chief Cetin Kiris (center, facing tour group) gives an overview of the D-Wave quantum computer and the HECC capabilities to students taking a computational physics class at California State University, East Bay.

POC: Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputing Division

Papers

- "**Spectra of Black Hole Accretion Models of Ultra-Luminous X-ray Sources**," R. Narayan, A. Sadowski, R. Soria, arXiv:1702.01158 [astro-ph.HE], February 3, 2017. * *https://arxiv.org/abs/1702.01158*
- "**Investigating Sources of Ozone over California using AJAX Airborne Measurements and Models: Assessing the Contribution from Long-Range Transport**," J.-M. Ryoo, M. Johnson, L. Iraci, E. Yates, W. Gore, Atmospheric Environment, February 7, 2017. * *http://www.sciencedirect.com/science/article/pii/S135223101730078X*
- "**Exploring the SDSS Data Set with Linked Scatter Plots. I. EMP, CEMP, and CV Stars**," D. Carbon, C. Henze, B. Nelson, The Astrophysical Journal: Supplement Series, vol. 228, no. 2, February 9, 2017. * *http://iopscience.iop.org/article/10.3847/1538-4365/228/2/19/meta*
- "**On the Origin of the Crescent-Shaped Distributions Observed by MMS at the Magnetopause**," G. Lapenta, et al., arXiv:1702.03550 [physics.space-ph], February 12, 2017. * *https://arxiv.org/abs/1702.03550*
- "**Heat-Shield Ablation Visualized Using Naphthalene Planar Laser-Induced Fluorescence**," C. Combs, N. Clemens, P. Danehy, S. Murman, Journal of Spacecraft and Rockets, February 15, 2017. * *http://arc.aiaa.org/doi/abs/10.2514/1.A33669*
- "**A General Probabilistic Approach for Quantitative Assessment of LES Combustion Models**," R. Johnson, arXiv:1702.05539 [physics.data-an], February 17, 2017. * *https://arxiv.org/abs/1702.05539*

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- "**How Anomalous Resistivity Accelerates Magnetic Reconnection**," H. Che, arXiv:1702.06109 [physics.space-ph], February 20, 2017. * *https://arxiv.org/abs/1702.06109*
- "**The Twist of the Draped Interstellar Magnetic Field Ahead of the Heliopause: A Magnetic Reconnection Driven Rotational Discontinuity**," M. Opher. J. Drake, M. Swisdak, B. Zieger, G. Toth, arXiv:1702.06178 [physics.space-ph], 20, 2017. * *https://arxiv.org/abs/1702.06178*
- "**A Fast Code for Channel Limb Radiances with Gas Absorption and Scattering in a Spherical Atmosphere**," J. Eluszkiewicz, et al., Journal of Quantitative Spectroscopy and Radiative Transfer, February 20, 2017. * *http://www.sciencedirect.com/science/article/pii/S0022407317301152*
- "**Supernova Driving. IV. The Star Formation Rate of Molecular Clouds**," P. Padoan, T. Haugbølle, Å. Nordlund, S. Frimann, arXiv:1702.07272 [astro-ph.GA], February 23, 2017. * *https://arxiv.org/abs/1702.07270*
- "**Deploying a Quantum Annealing Processor to Detect Tree Cover in Aerial Imagery of California**," E. Boyda, S. Basu, S. Ganguly, A. Michaelis, S. Mukopadhyay, R. Nemani, PLOSOne, February 27, 2017. * *http://journals.plos.org/plosone/article?id=10.1371/journal.pone.0172505*

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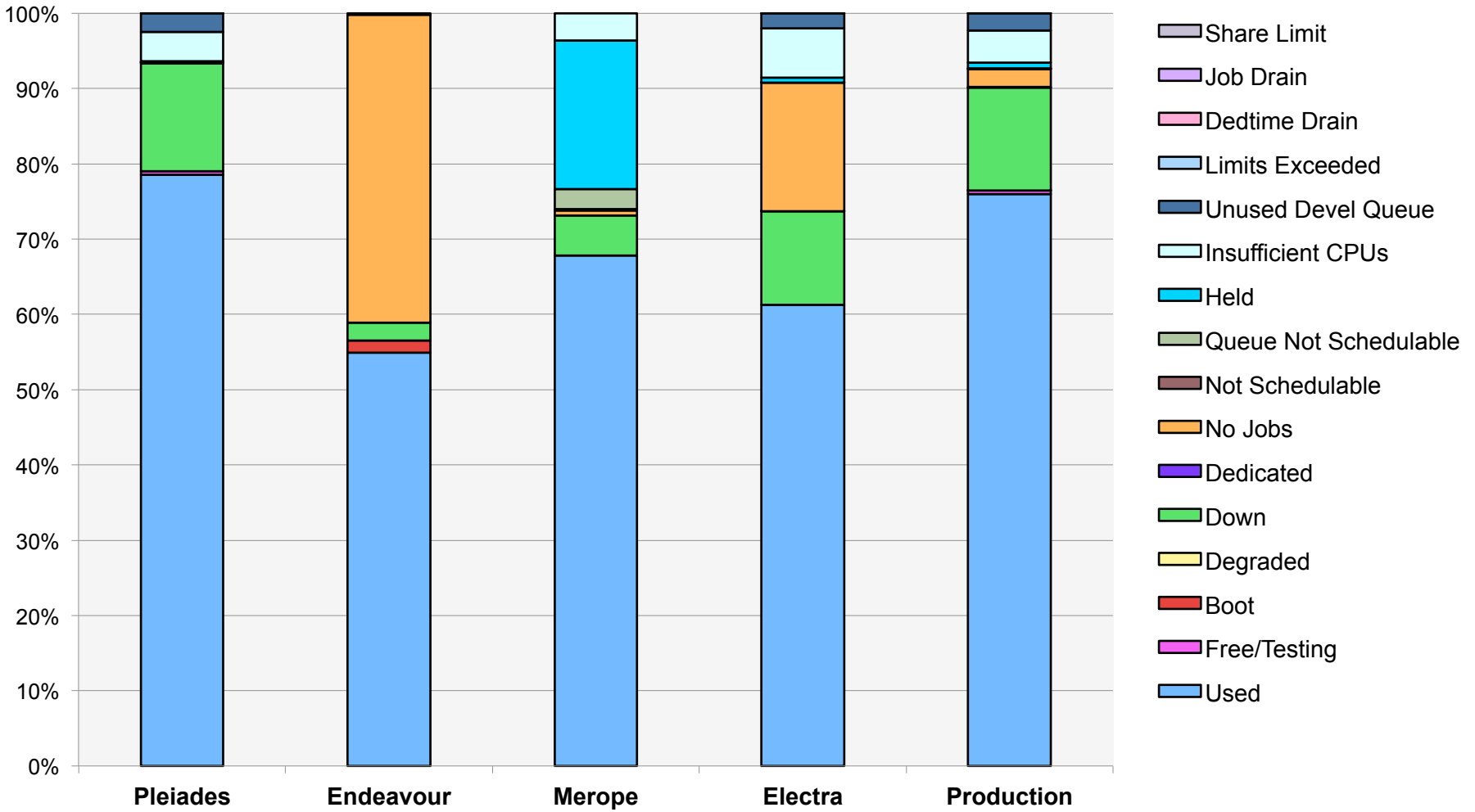
News & Events

- **Managing Energy Efficiency at NASA**, *Scientific Computing World,* February 1, 2017—Robert Roe interviews Bill Thigpen and discusses how NAS is optimizing energy efficiency and water usage to maximize the facility's potential to deliver computing services to the HECC user community. *https://www.scientific-computing.com/feature/managing-energy-efficiency-nasa*
- **Our Supermassive Black Hole Could Be 'Supercharging' Stars' Magnetism**, *Seeker,* February 2, 2017—Using the NAS facility's high-end computing resources, astronomers at the Harvard-Smithsonian Center for Astrophysics have—for the first time—been able to include the magnetic fields of stars in computer simulations where a star is "pulled apart and stretched," giving a clue about how the stars in the center of our galaxy respond to straying too close to a monster black hole. *http://www.seeker.com/supermassive-black-hole-stars-magnetism-computer-simulations-2233559927.html*
- **NASA Ames Kicks off Pathfinding Modular Supercomputing Facility**, *NAS Feature Story*, February 16, 2017—NASA's concept for an innovative modular supercomputing facility (MSF) has the potential to save million gallons of water a year while providing additional resources for agency science and engineering projects. *https://www.nas.nasa.gov/publications/articles/feature_MSF_Kickoff.html*
  - **NASA Saves Energy and Water with New Modular Supercomputing Facility**, *NASA Ames*, February 17, 2017. *https://www.nasa.gov/ames/feature/nasa-ames-kicks-off-pathfinding-modular-supercomputing-facility*
  - **NASA Saves Energy and Water with New Modular Supercomputing Facility**, *Phys.Org*, February 20, 2017. *https://phys.org/news/2017-02-nasa-energy-modular-supercomputing-facility.html*
  - **NASA Saves Energy, Water with New Modular Supercomputing Facility**, *Energy Manager Today*, February 23, 2017. *http://www.energymanagertoday.com/nasa-saves-energy-water-modular-supercomputer-0167595/*
  - **NASA Buys into Modular Supercomputing with New Facility that Saves Energy and Water**, *TOP500*, February 24, 2017. *https://www.top500.org/news/nasa-buys-into-modular-supercomputing-with-new-facility-that-saves-energy-and-water/*
  - **Modular Supercomputers: Smaller Environmental Footprint, Greater Flexibility**, *GCN*, February 27, 2017. *https://gcn.com/articles/2017/02/27/modular-supercomputer.aspx*

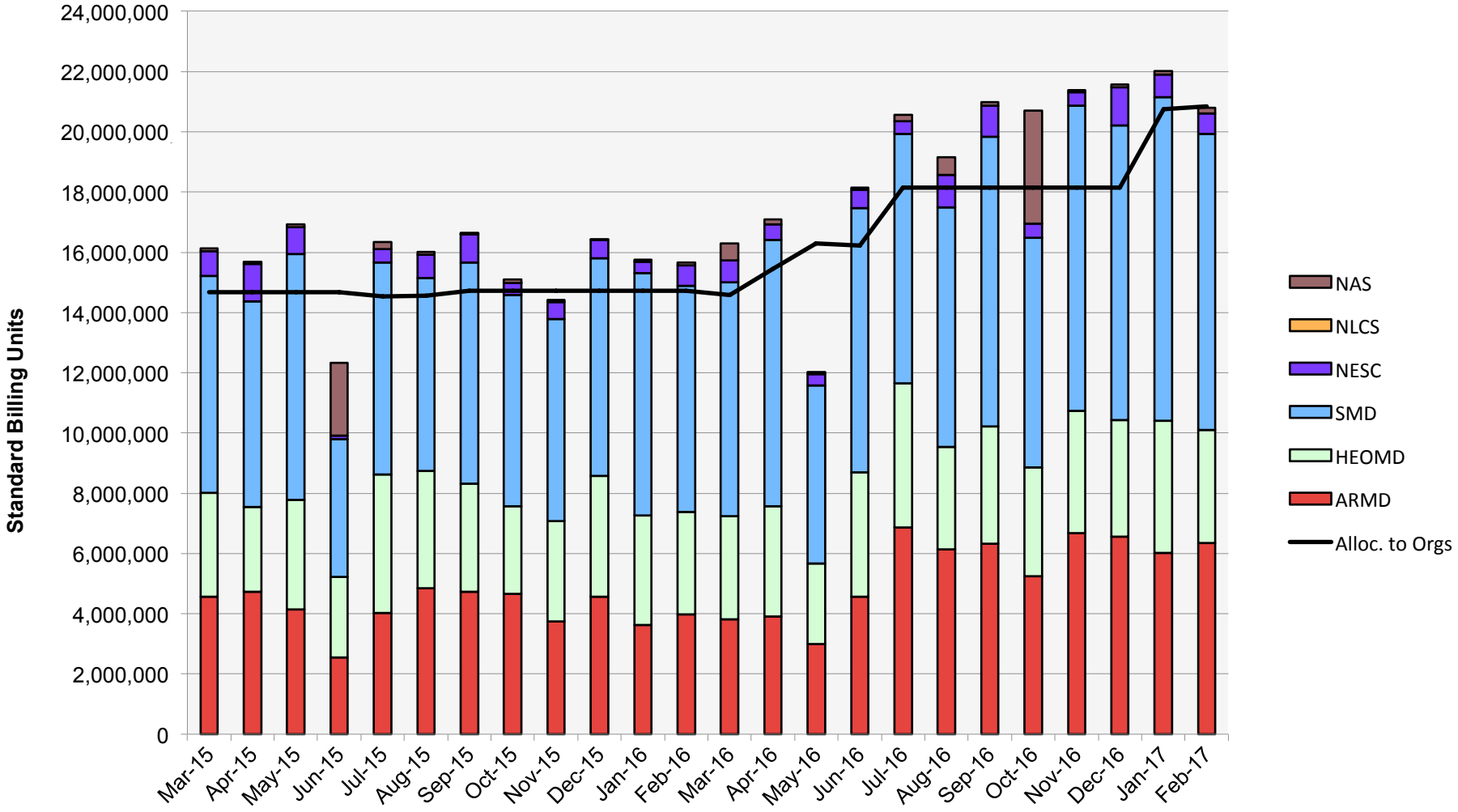
News & Events (cont.)

- **When Rocket Science Meets X-ray Science**, *Lawrence Berkeley National Laboratory News Release,* February 21, 2017—First in a four-part series by Lawrence Berkeley Lab's Glenn Roberts Jr. focuses on a partnership between NASA and the Lab to explore spacecraft thermal protection materials in microscale detail. Analysis and simulations were produced using the Pleiades supercomputer, and visualizations were produced by HECC visualization experts.
  https://newscenter.lbl.gov/2017/02/21/space-rocket-science-meets-x-ray-science/
  - **The Heat is On**, *LBNL*, February 22, 2017—Part 2 in the four-part series.
    http://newscenter.lbl.gov/2017/02/22/building-heat-shield-mars-mission/
  - **A New Paradigm in Parachute Design**, February 23, 2017—Part 3 in the four-part series.
    https://newscenter.lbl.gov/2017/02/23/new-paradigm-parachute-design/
  - **Getting to Know Meteors Better**, February 24, 2017—Part 4in the four-part series.
    https://newscenter.lbl.gov/2017/02/24/getting-know-meteors-better/

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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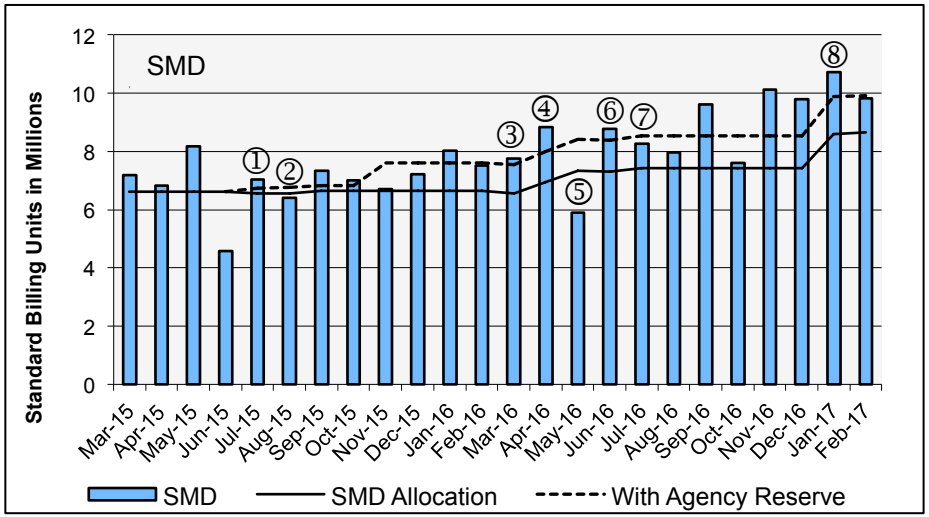
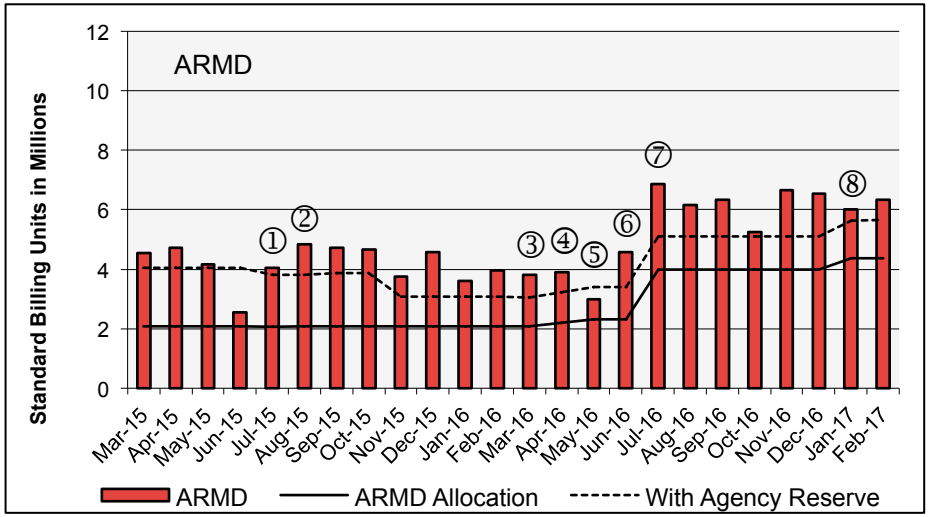
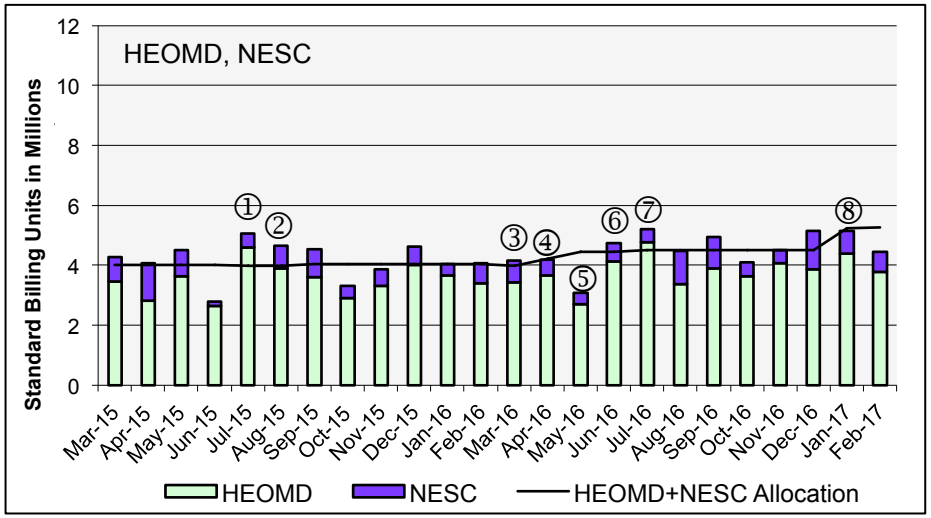
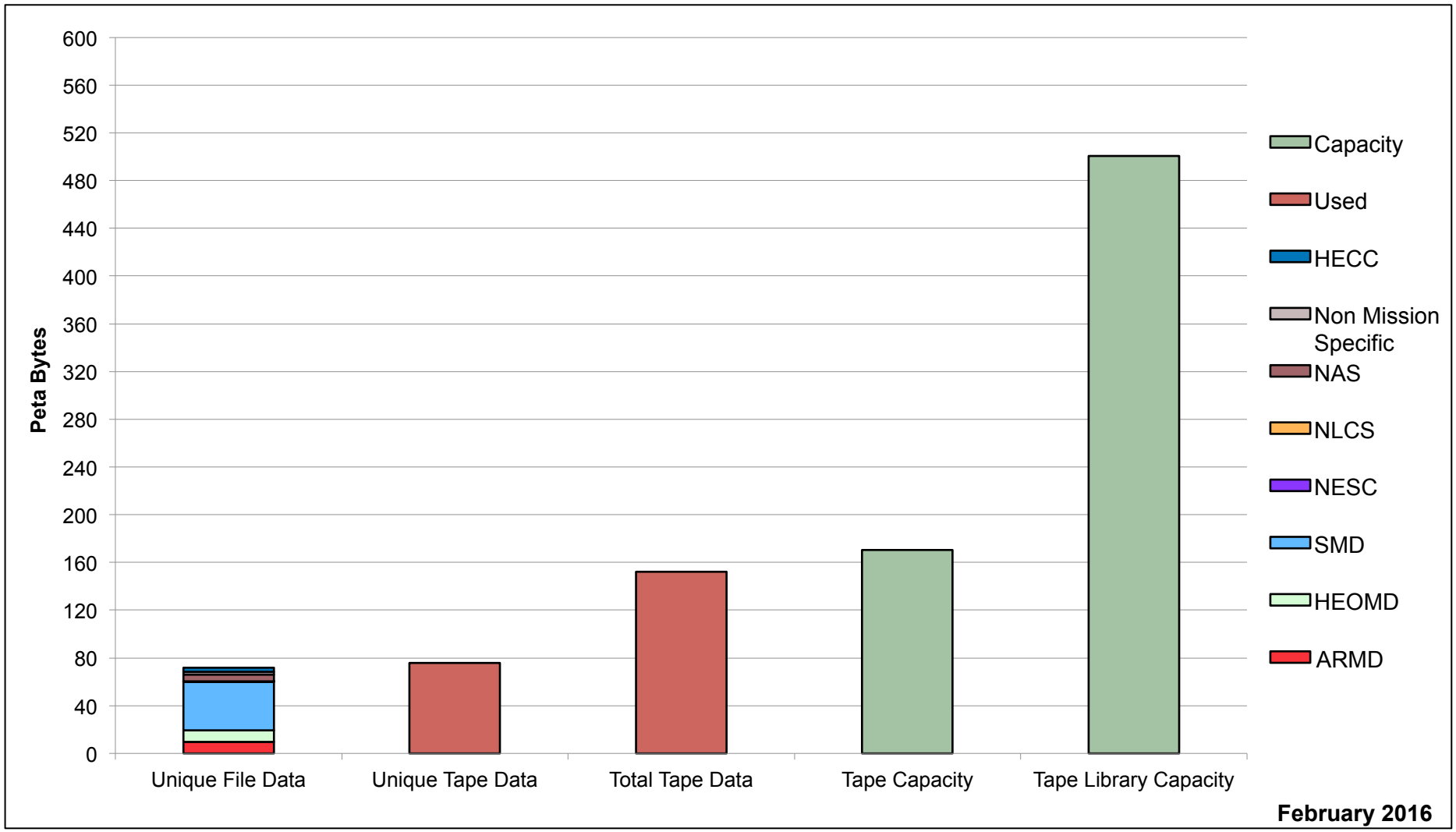






① 7 Nehalem ½ racks retired from Merope
② 7 Westmere ½ racks added to Merope
③ 16 Westmere racks retired from Pleiades
④ 10 Broadwell racks added to Pleiades
⑤ 4 Broadwell racks added to Pleiades
⑥ 14 (All) Westmere racks retired from Pleiades
⑦ 14 Broadwell Racks added to Pleiades
⑧ 16 Electra Broadwell Racks in Production, 12 Westmere 1/2 racks added to Merope

Tape Archive Status



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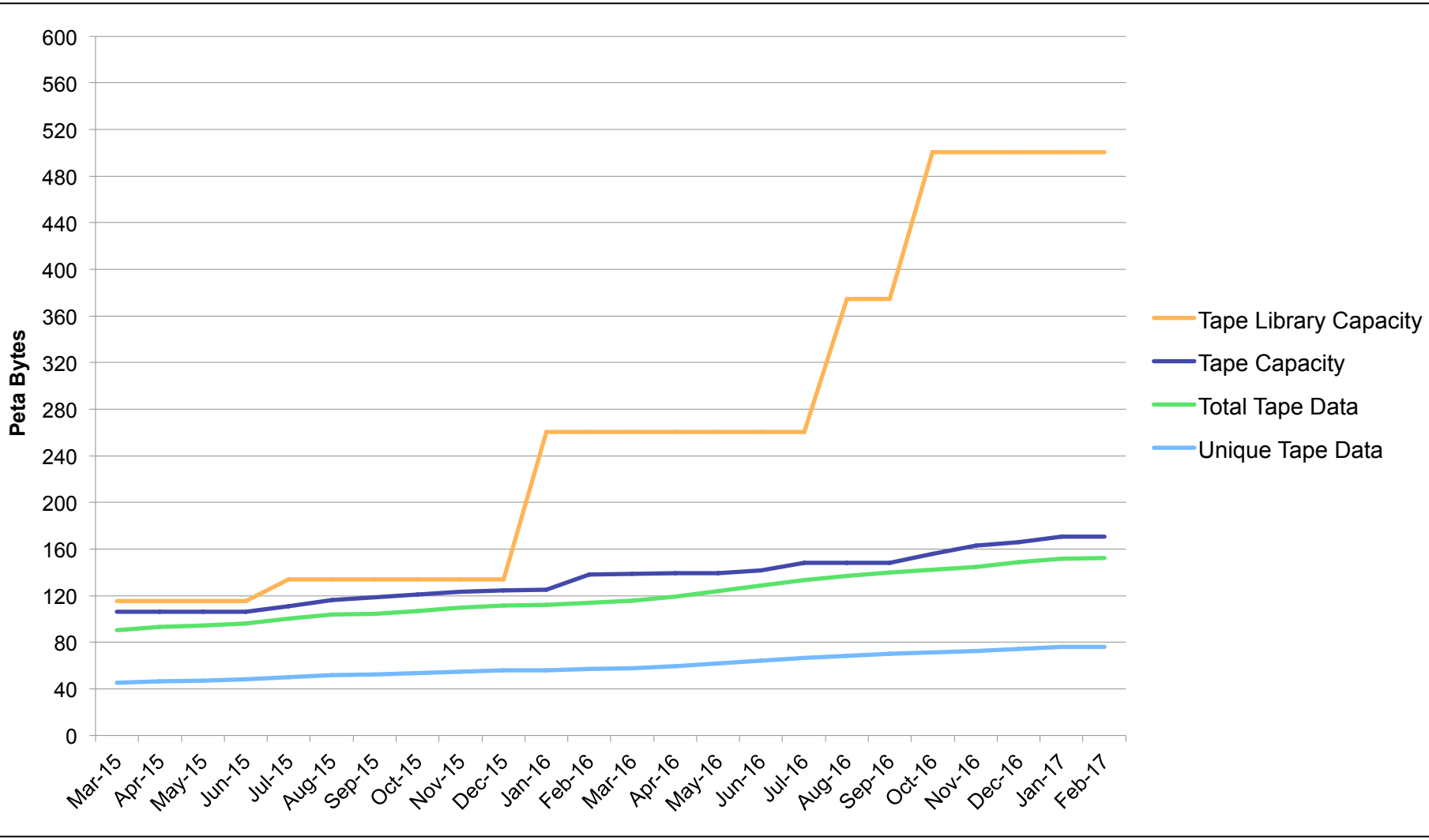
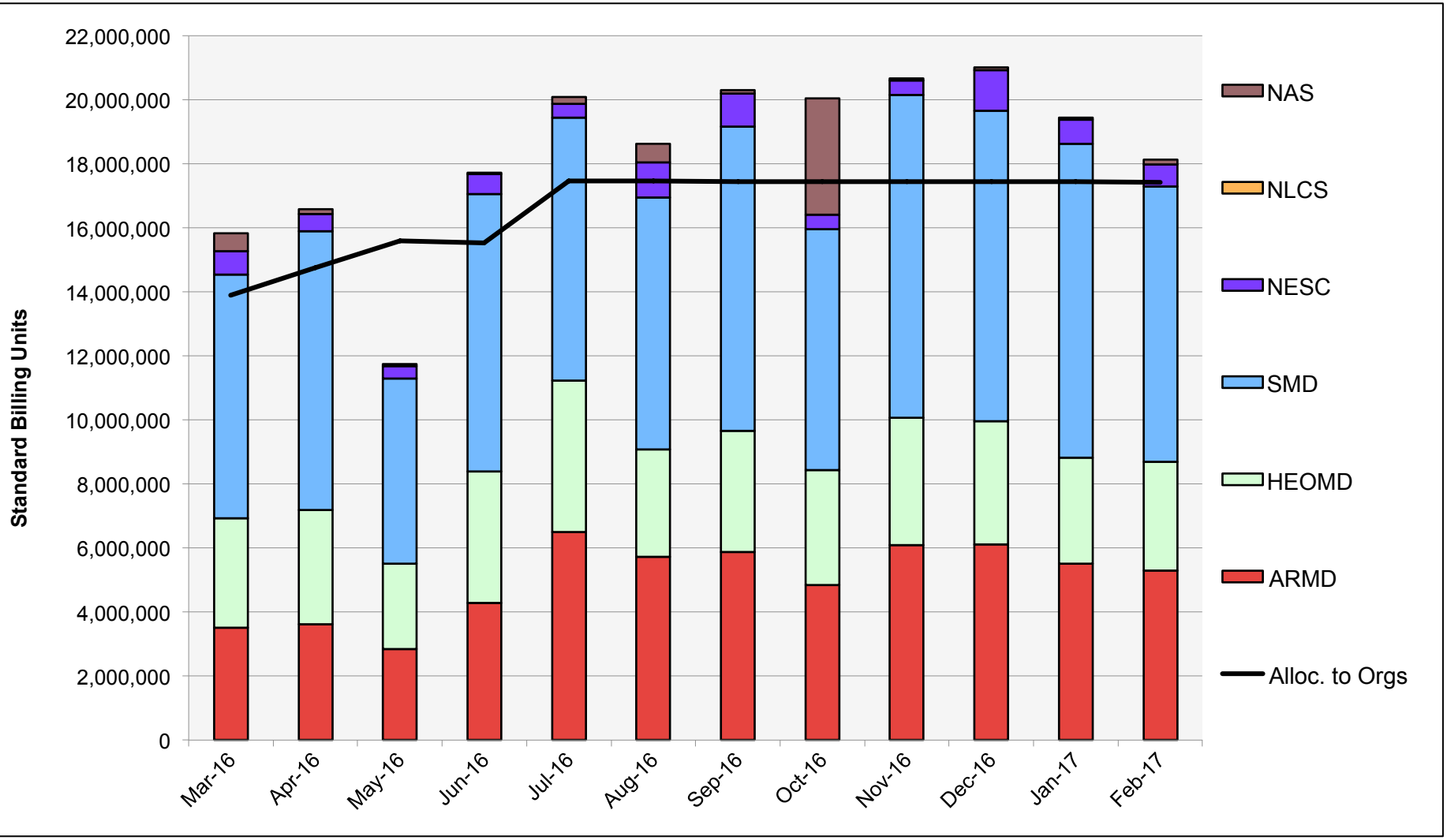
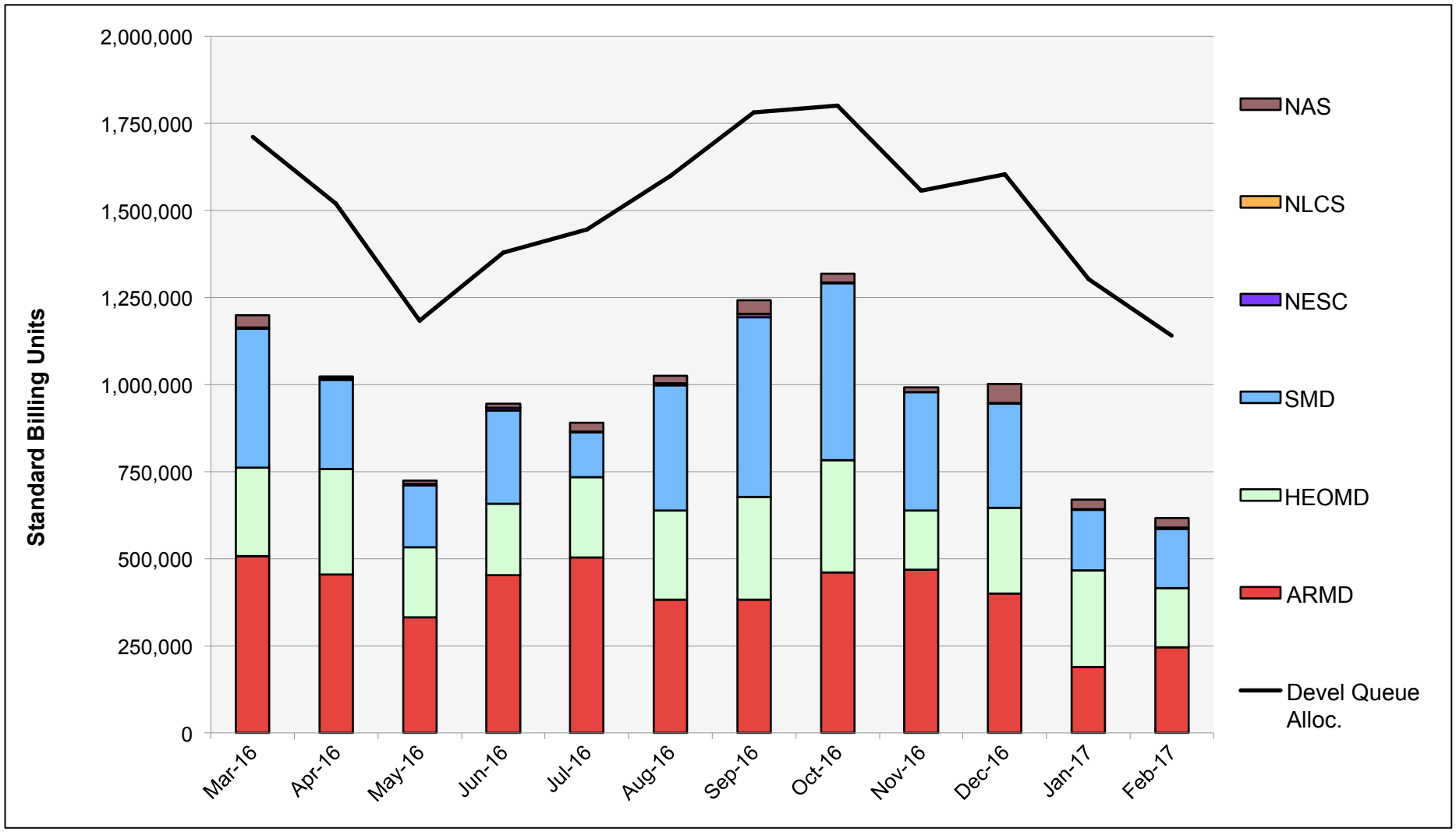


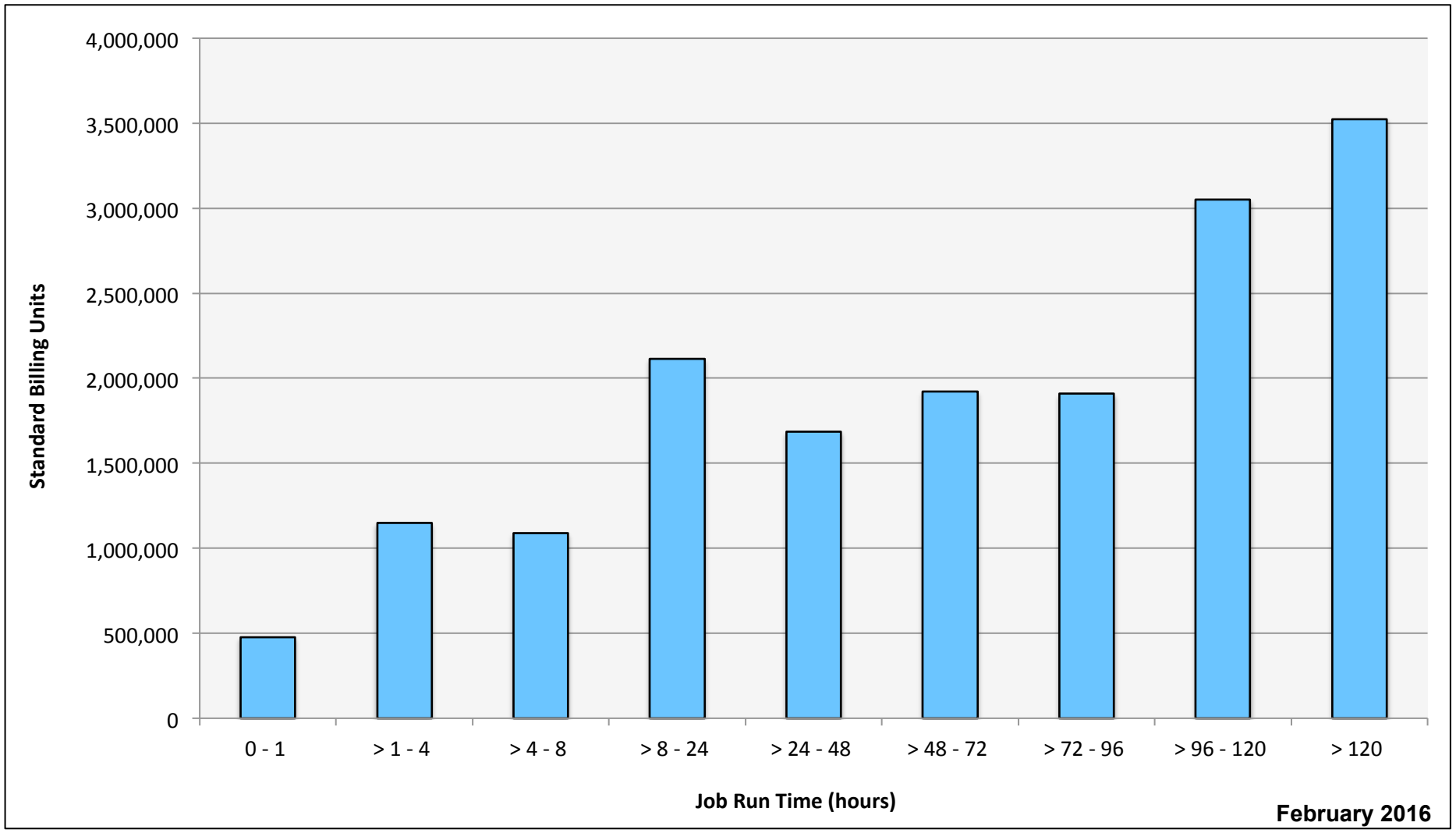
Pleiades:
SBUs Reported, Normalized to 30-Day Month



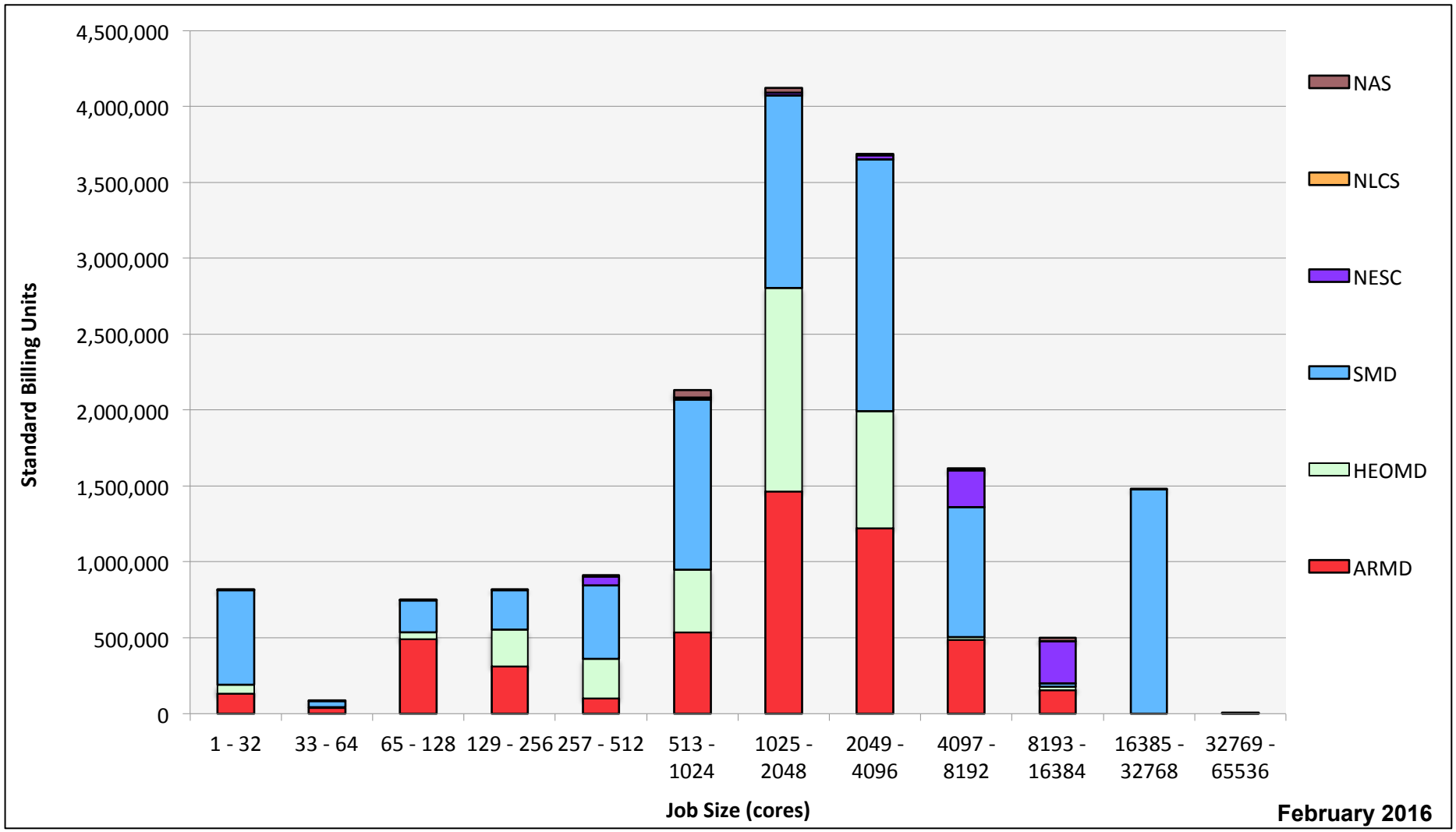
Pleiades:
Devel Queue Utilization



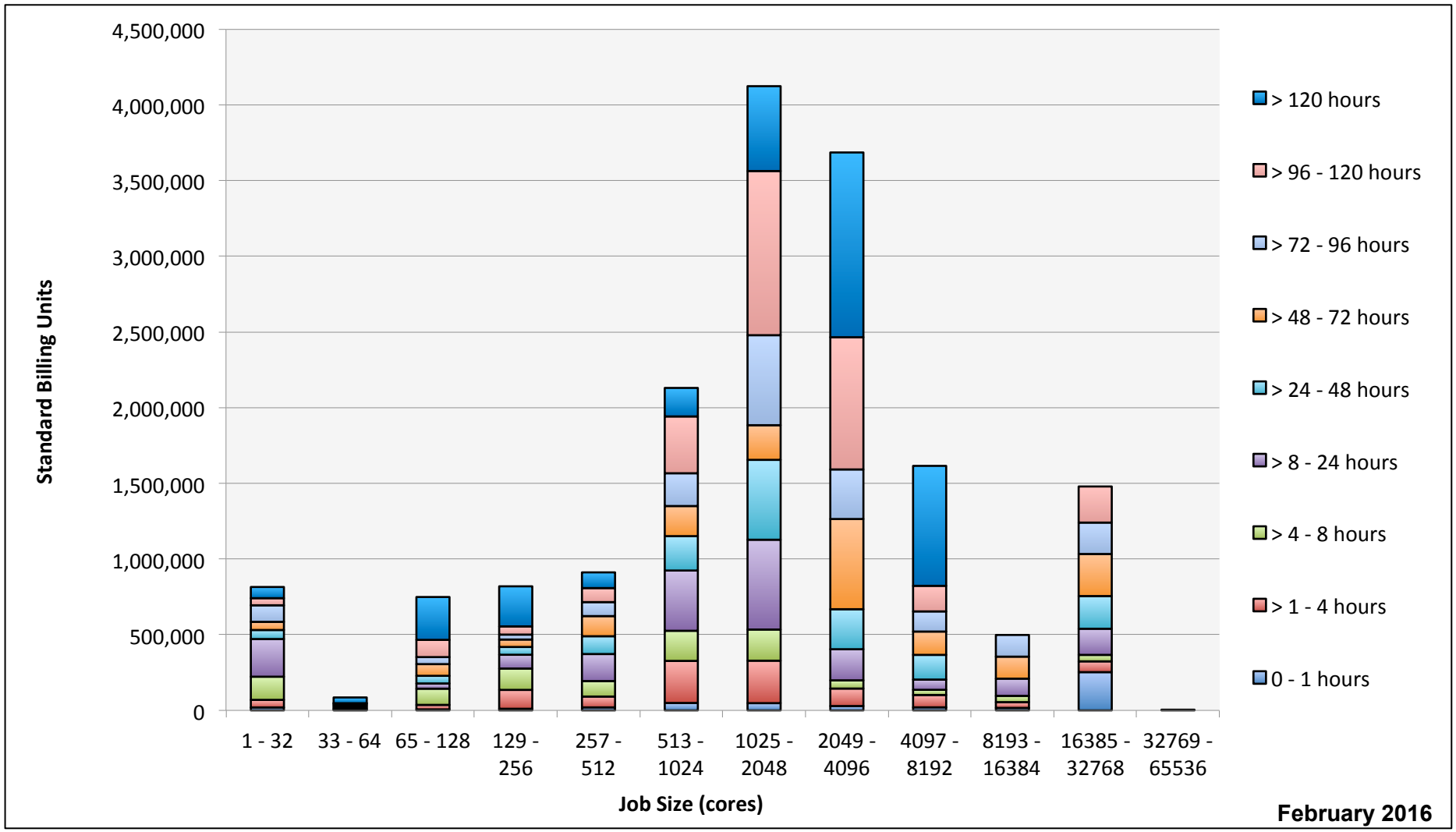
Pleiades:
Monthly Utilization by Job Length



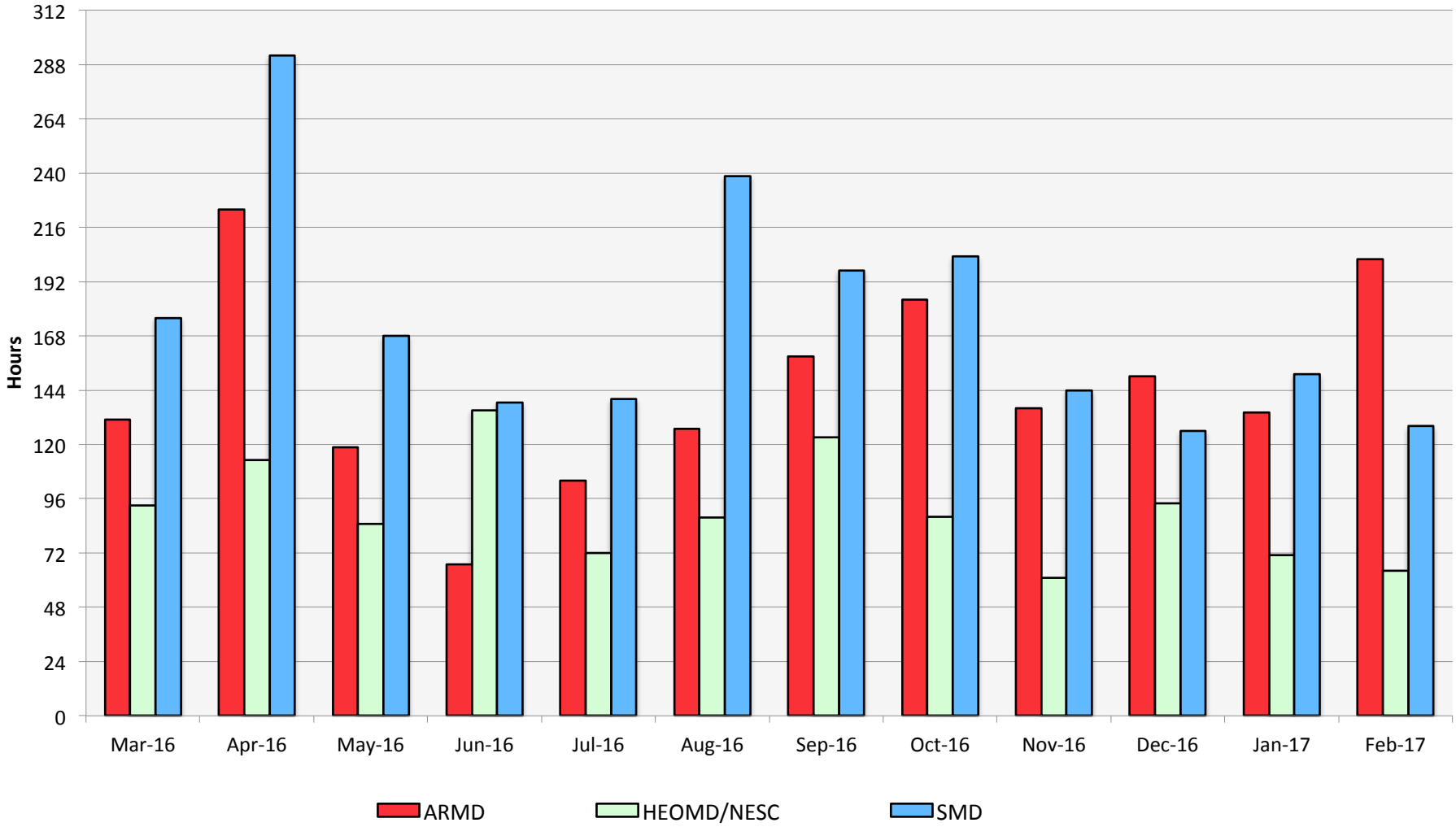
Pleiades:
Monthly Utilization by Size and Mission



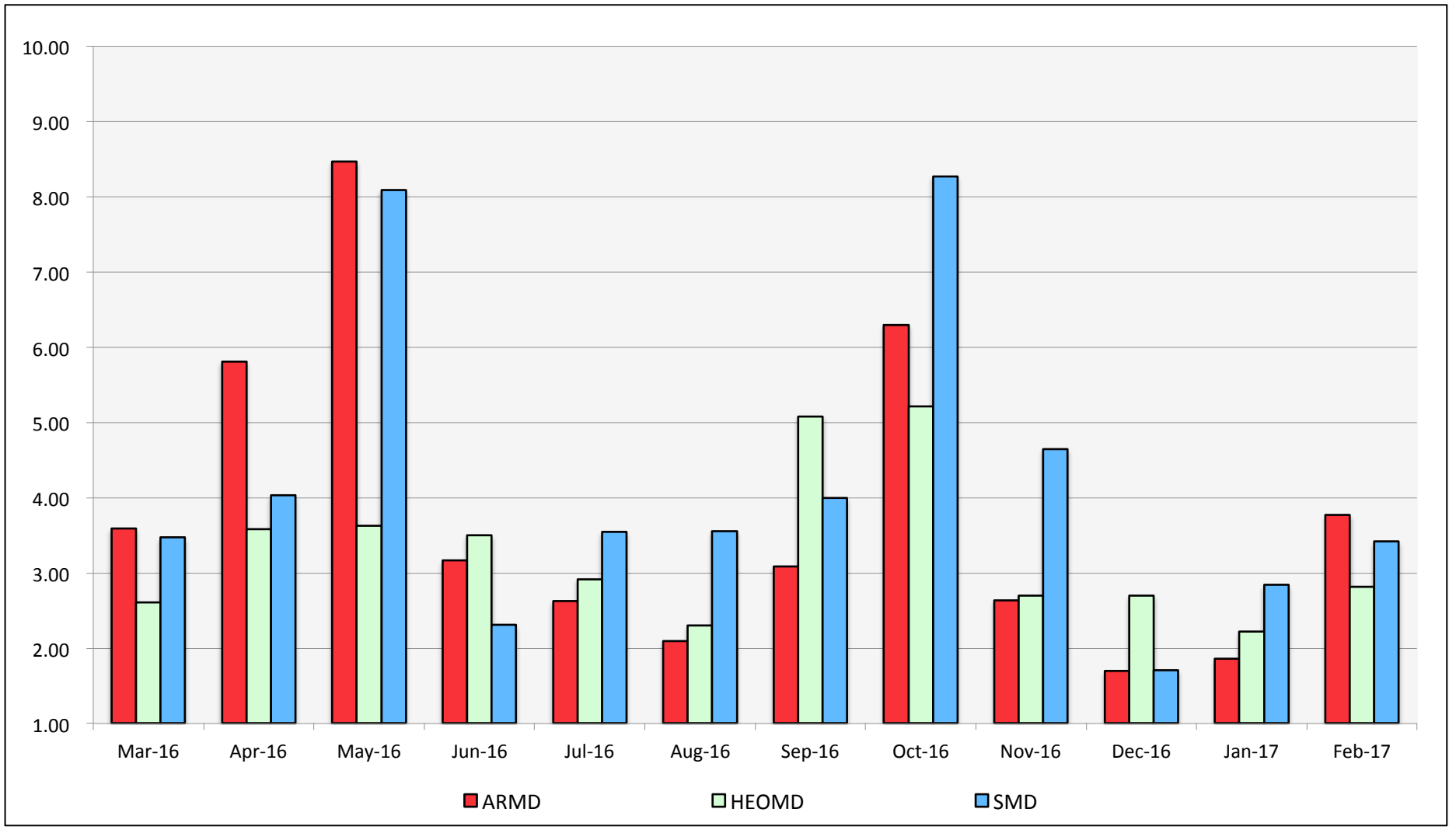
Pleiades:
Monthly Utilization by Size and Length



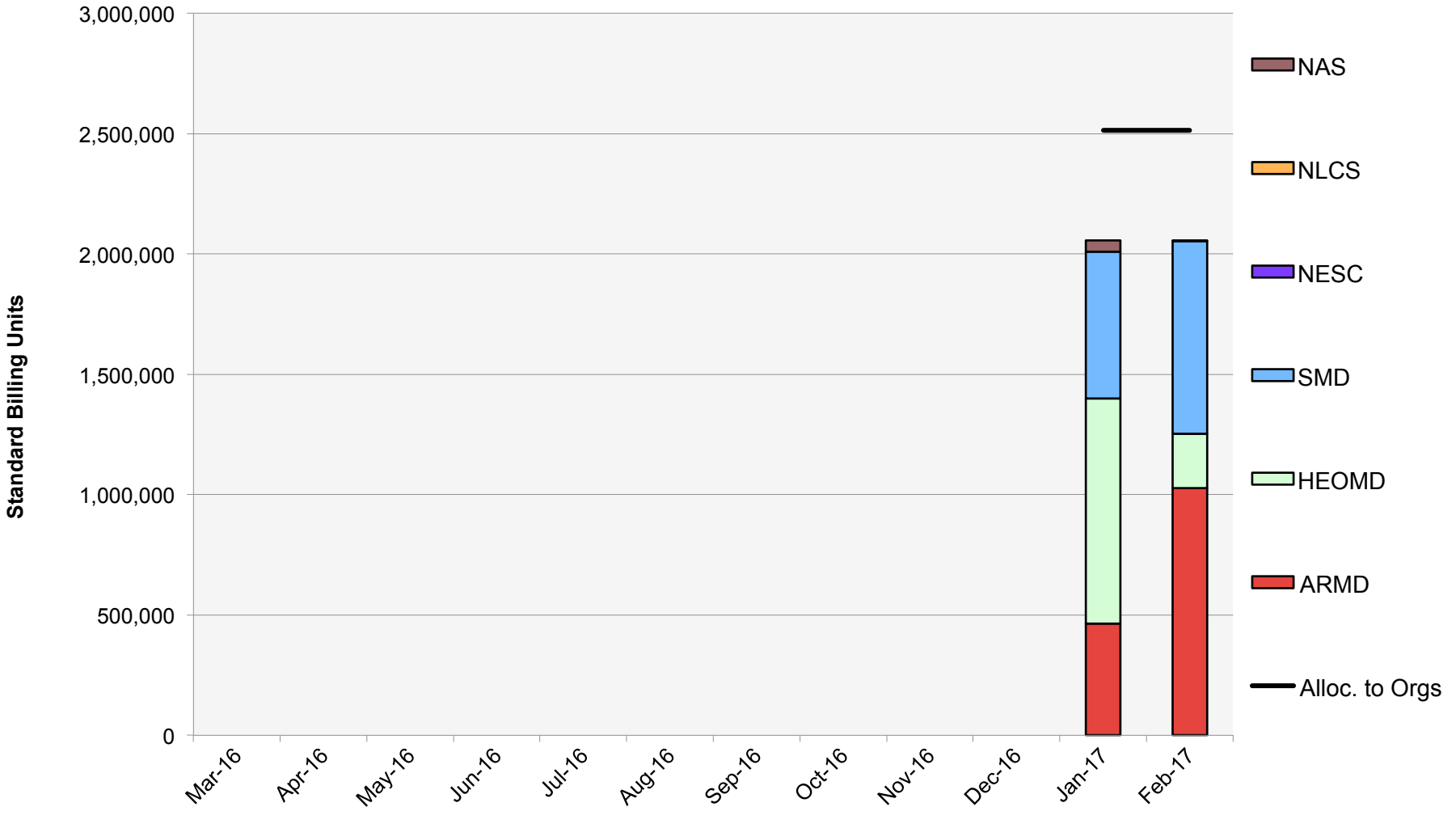
Pleiades:
Average Time to Clear All Jobs



Pleiades:
Average Expansion Factor



Electra:
SBUs Reported, Normalized to 30-Day Month



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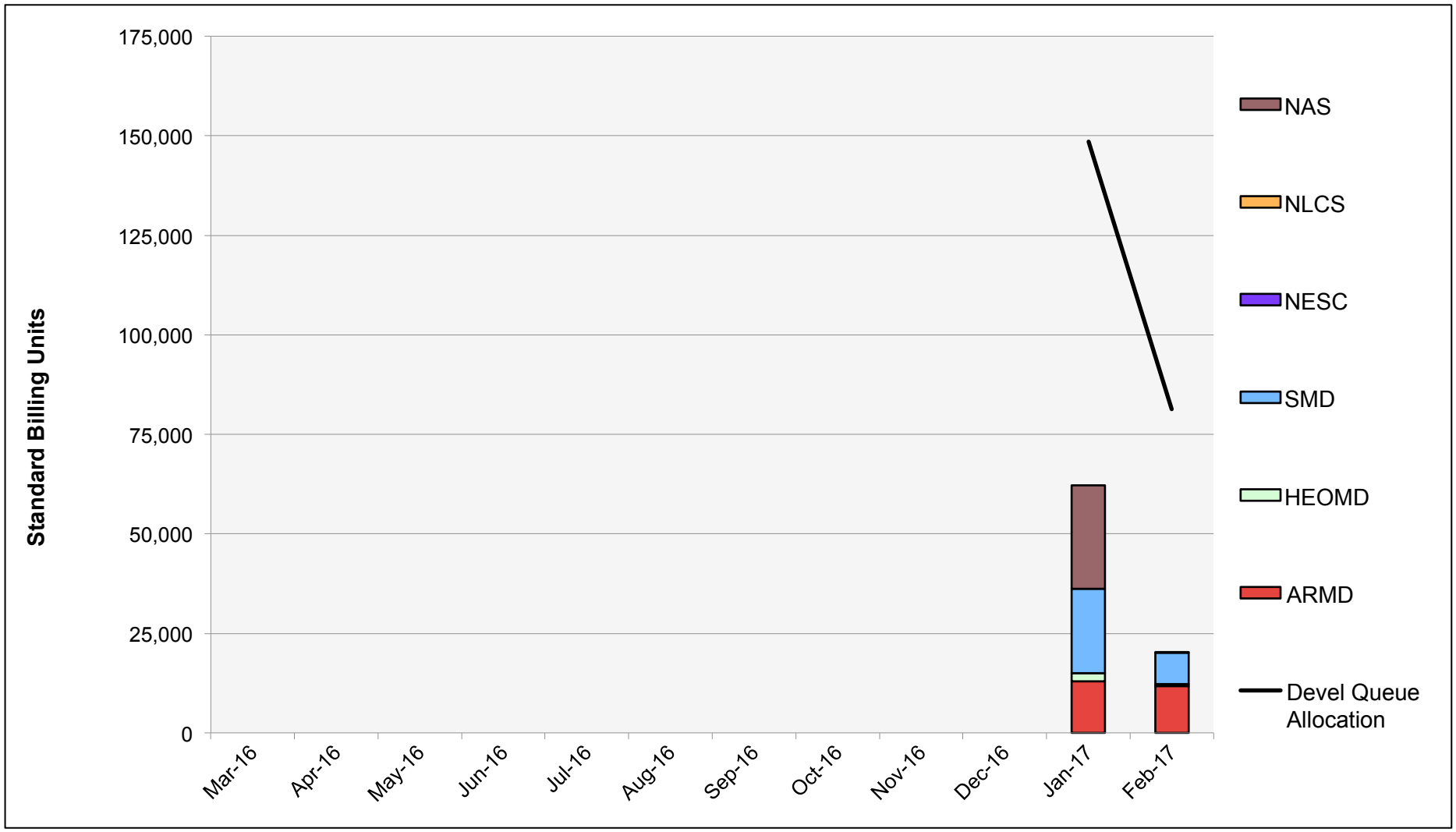
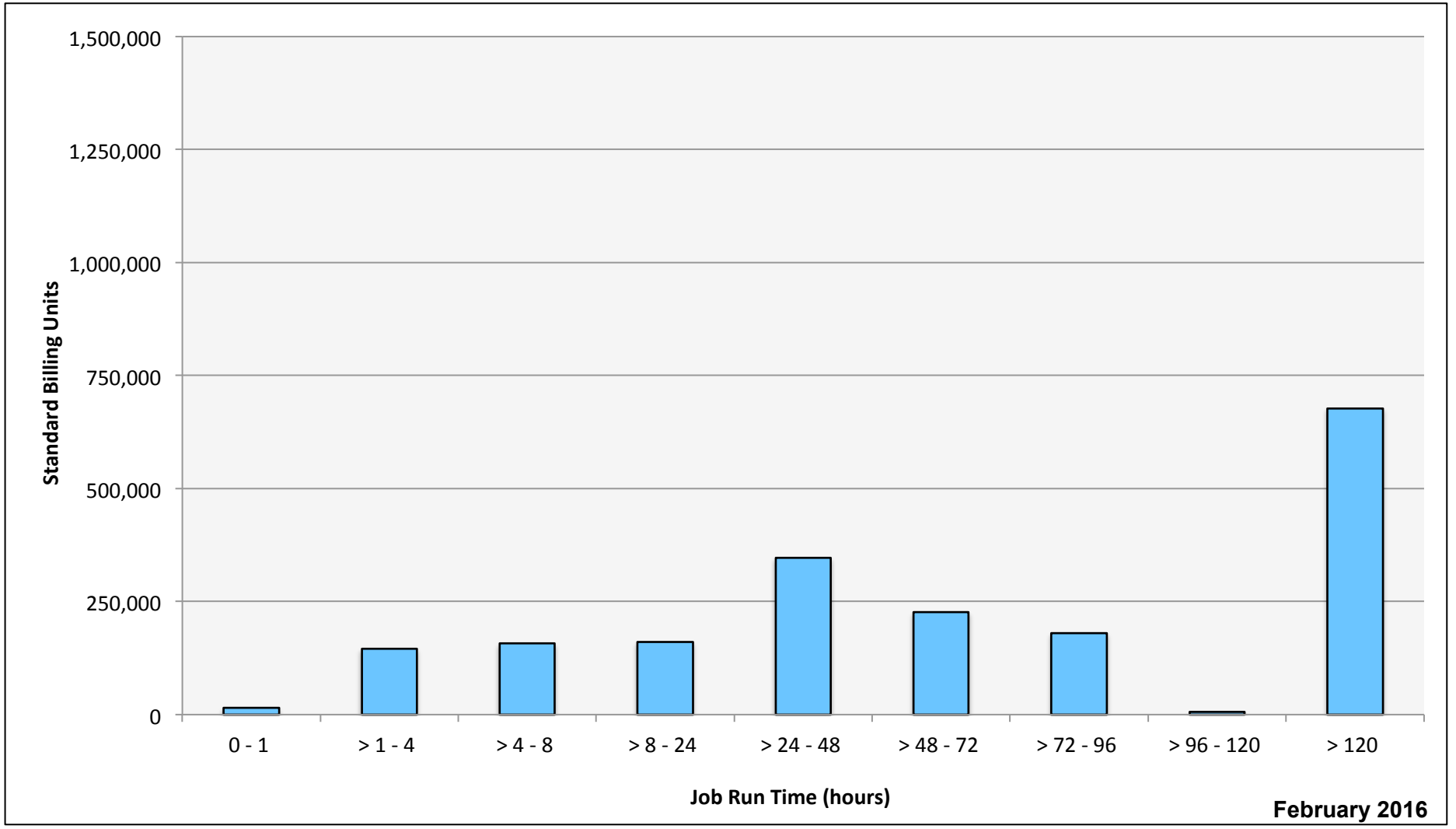
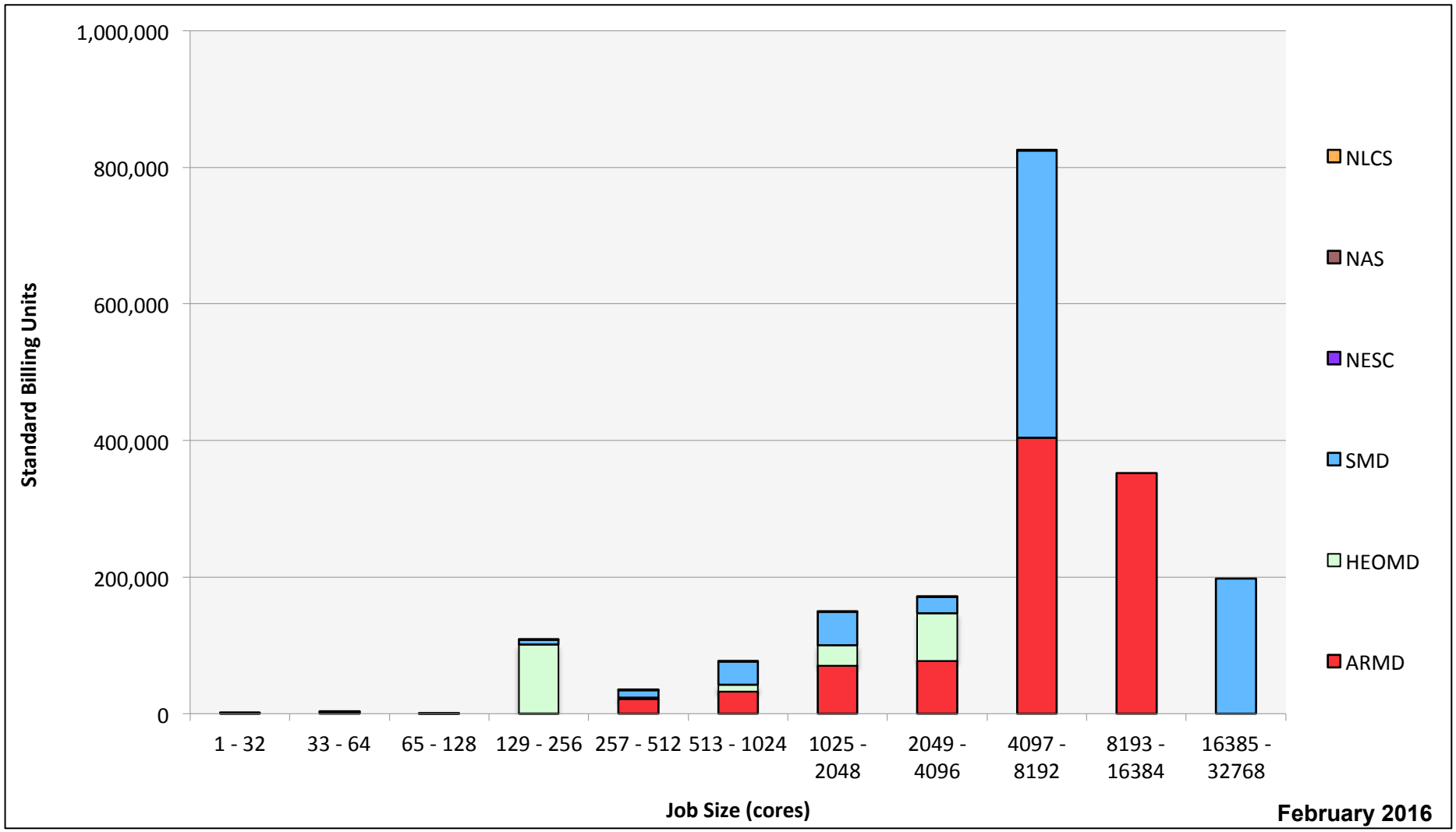
Devel Queue Utilization



Electra:
Monthly Utilization by Job Length



Electra:
Monthly Utilization by Size and Mission



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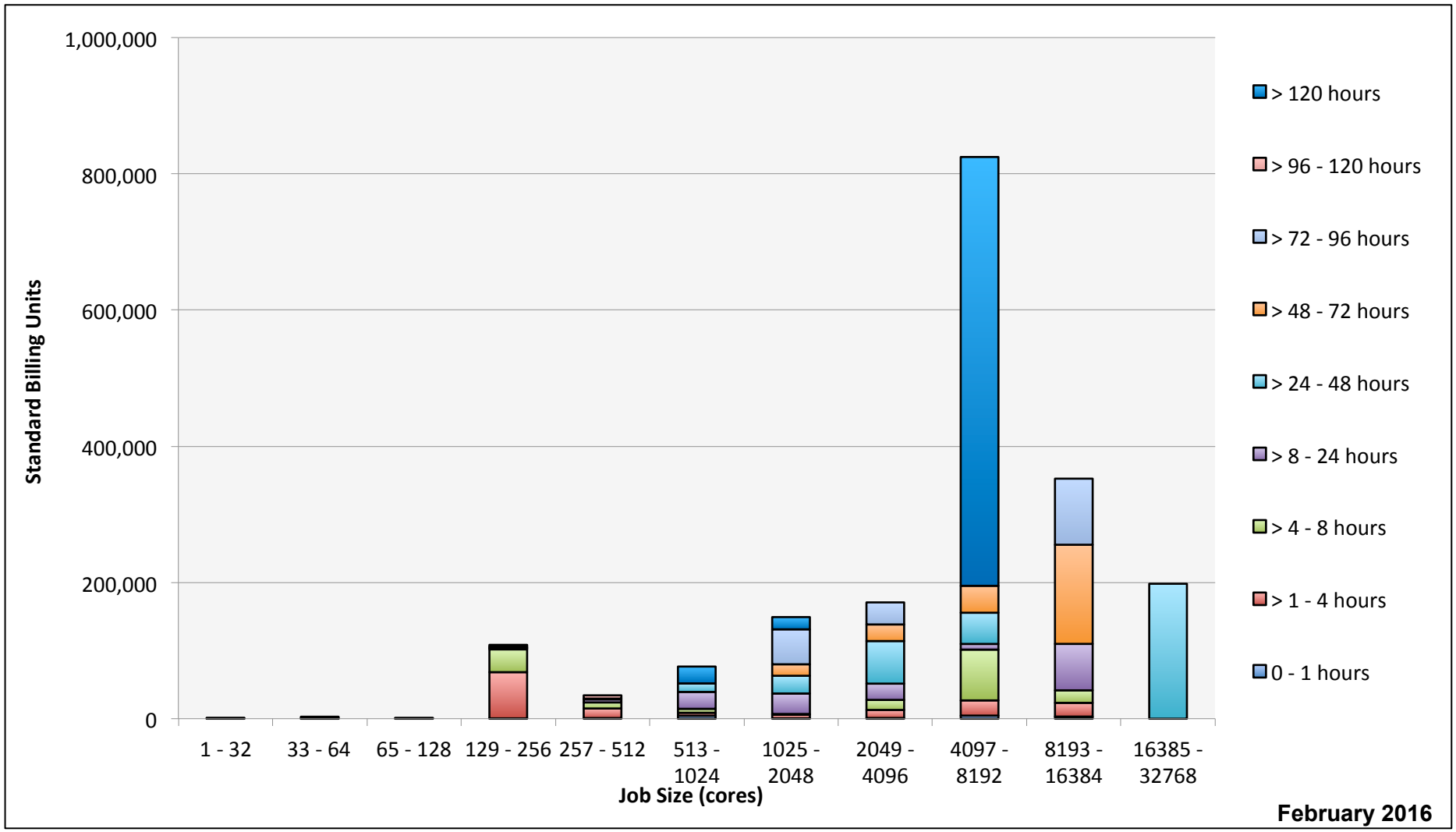

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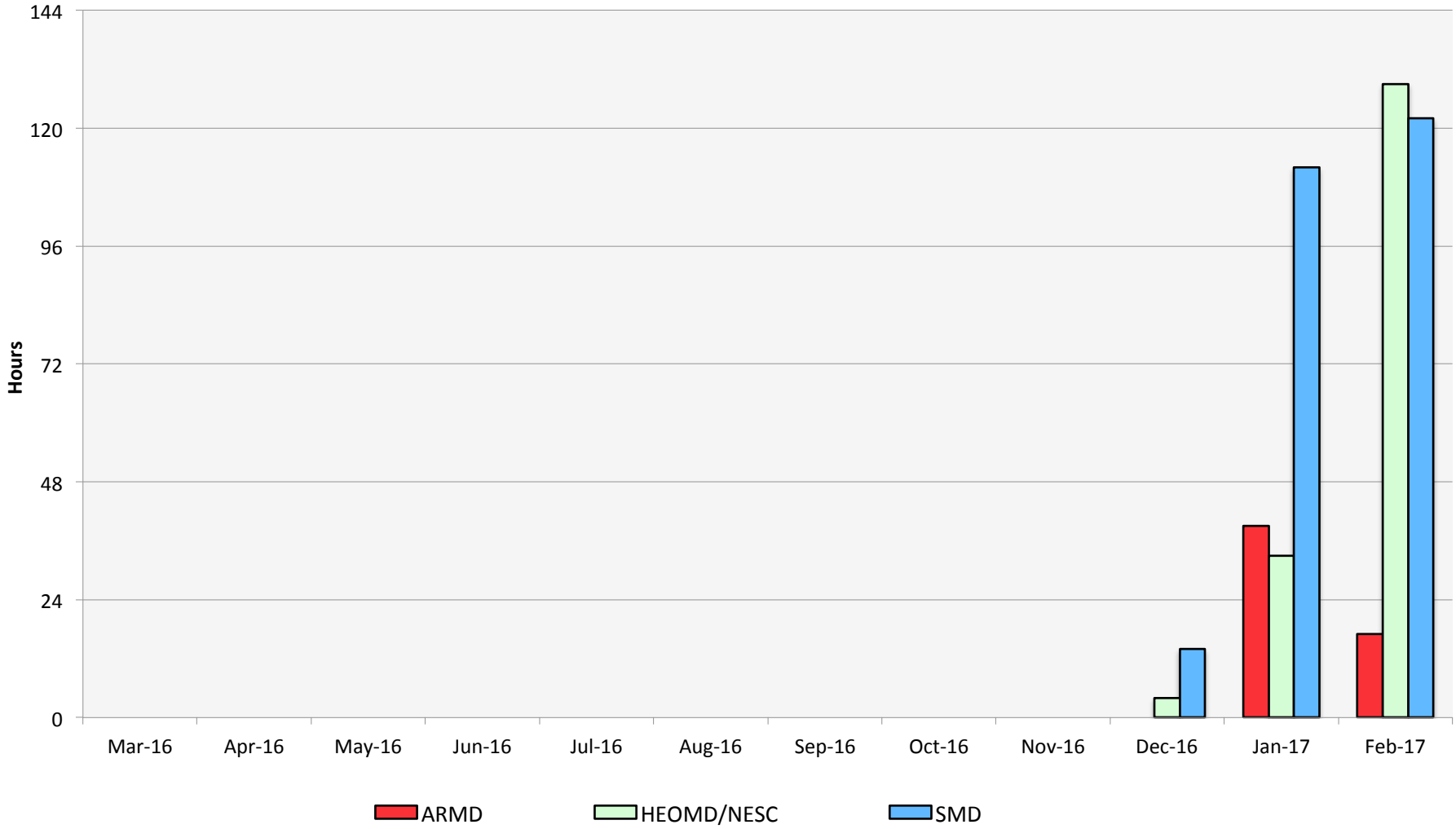
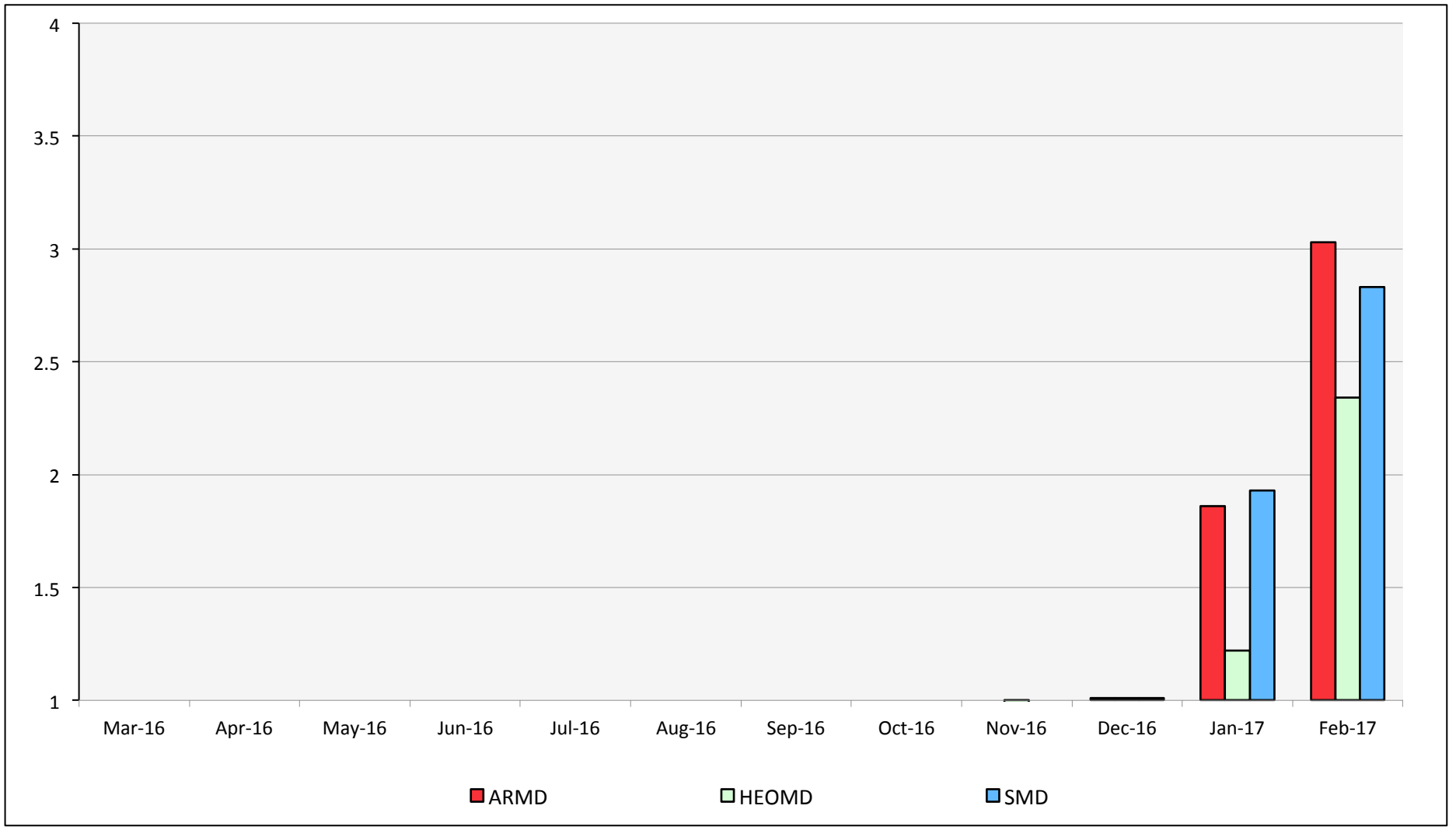
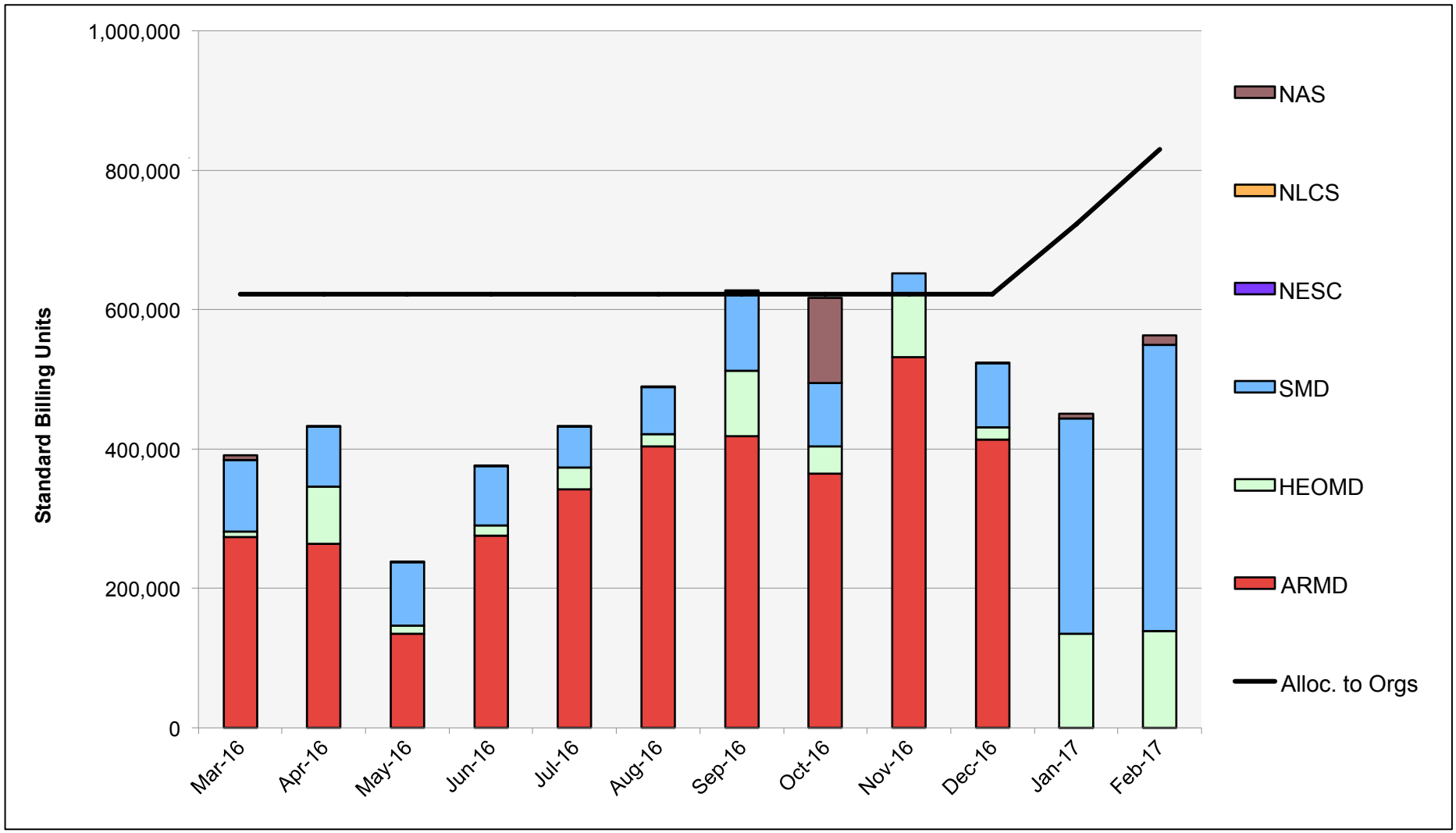


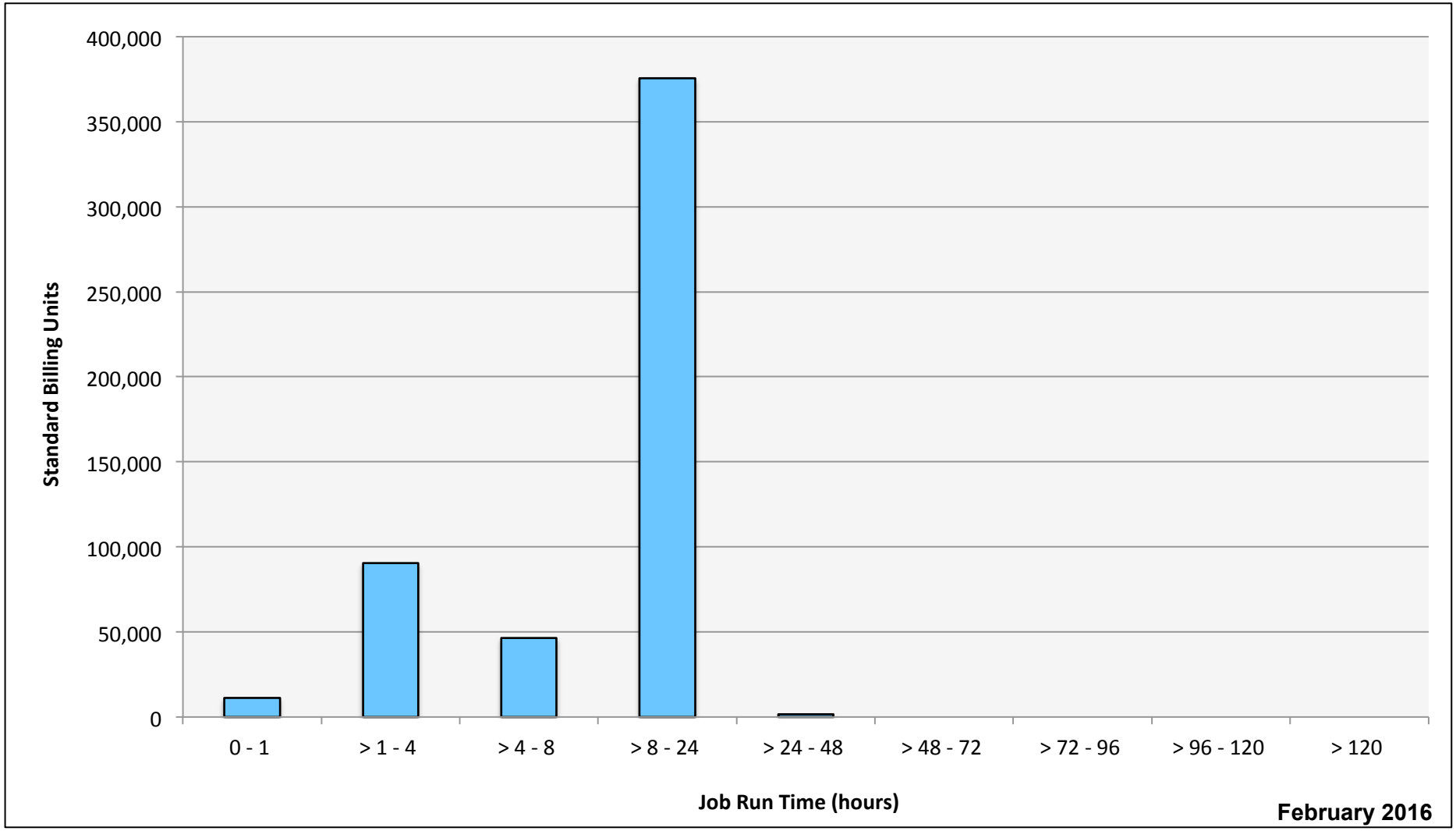
Electra:
Average Expansion Factor



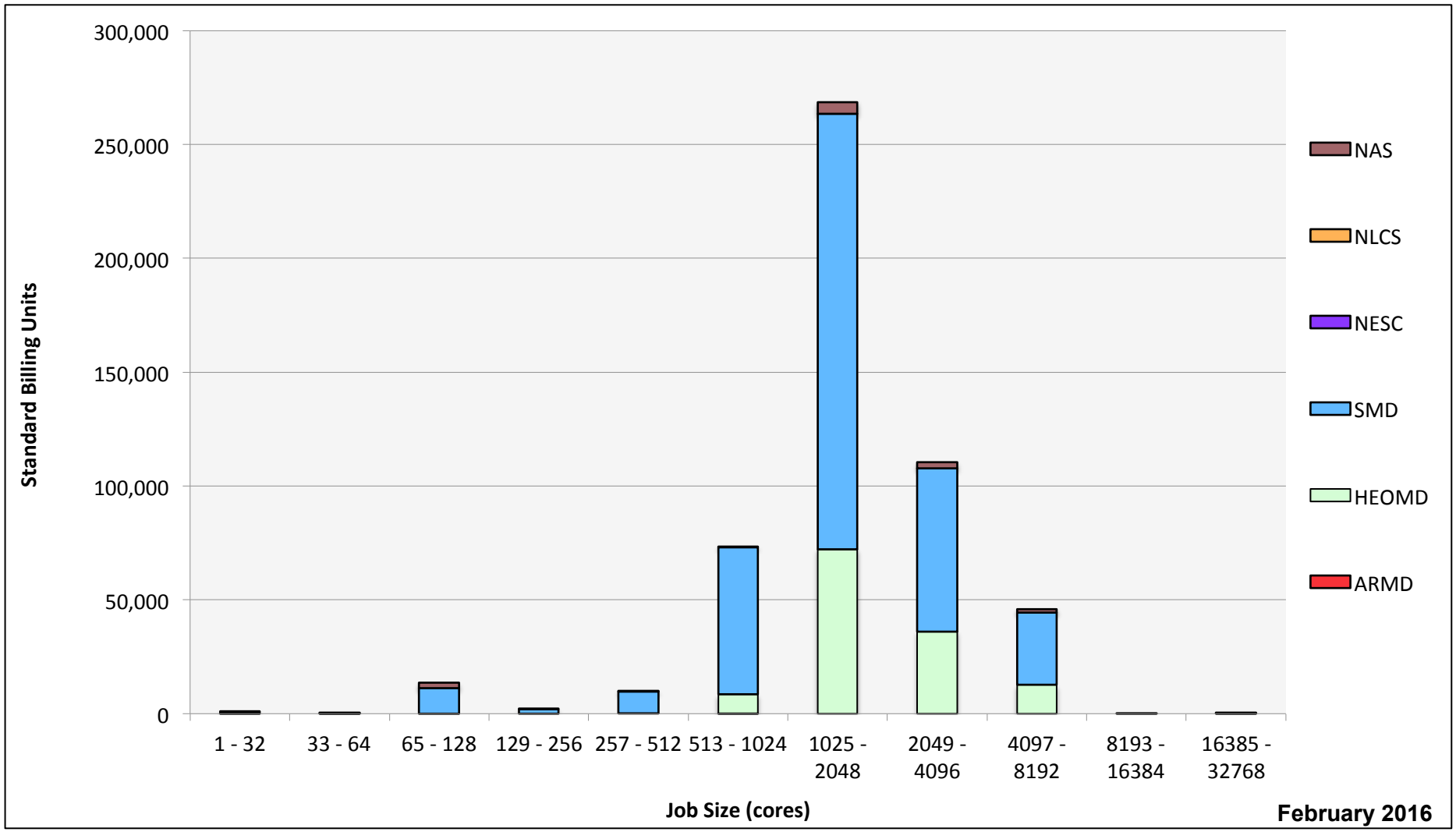
Merope:
SBUs Reported, Normalized to 30-Day Month



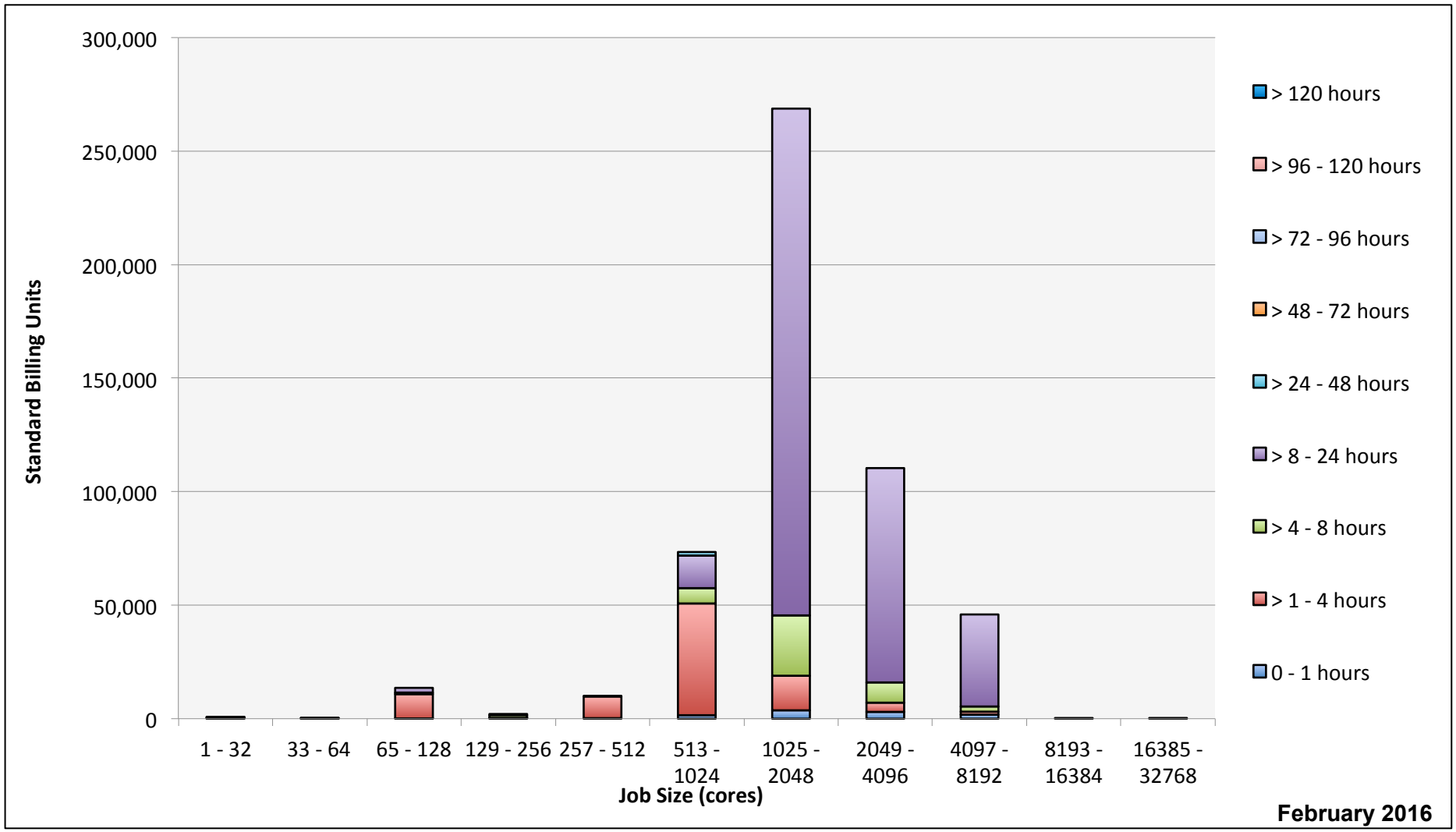
Merope:
Monthly Utilization by Job Length



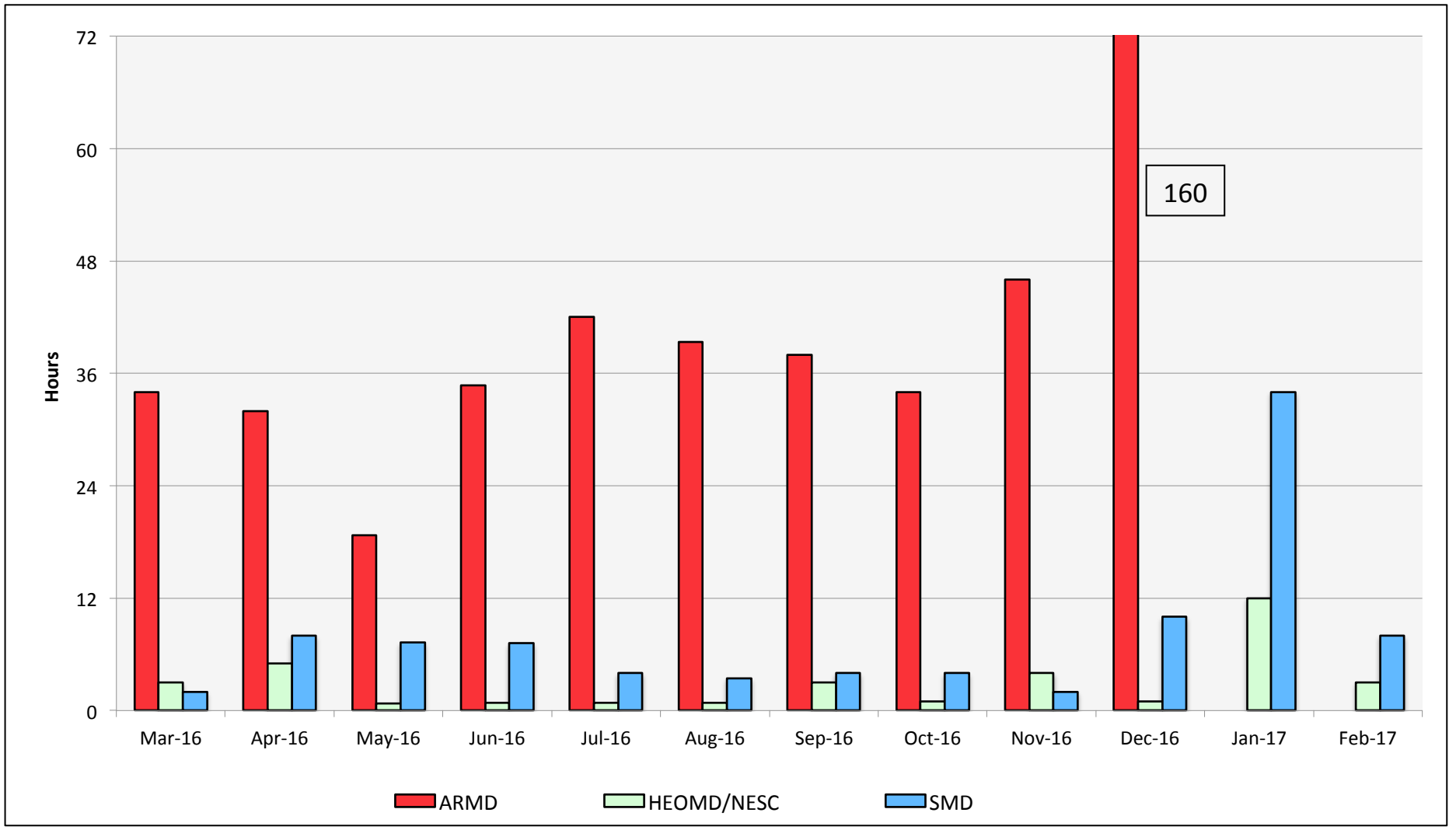
Merope:
Monthly Utilization by Size and Mission



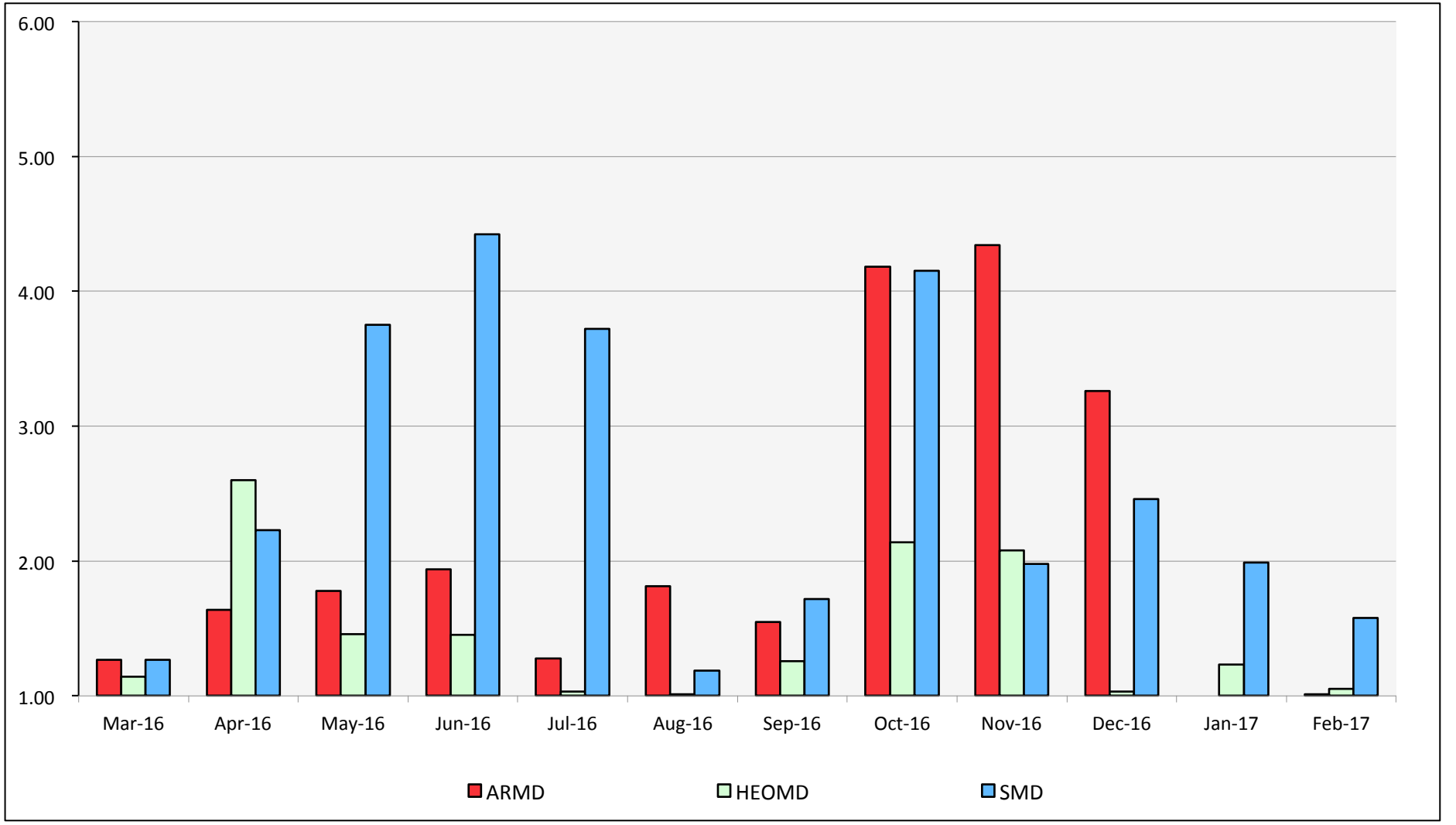
Merope:
Monthly Utilization by Size and Length



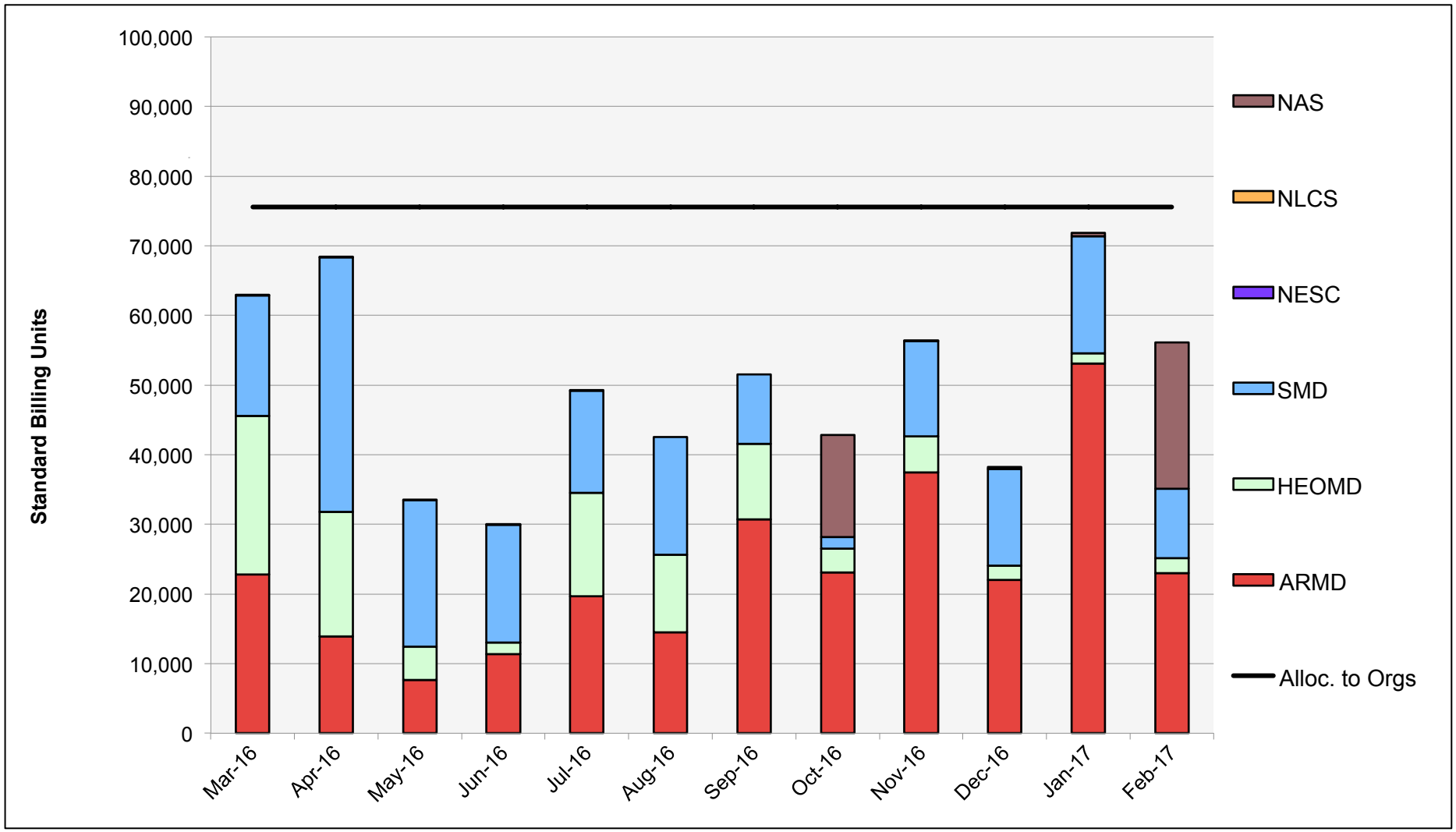
Merope:
Average Time to Clear All Jobs



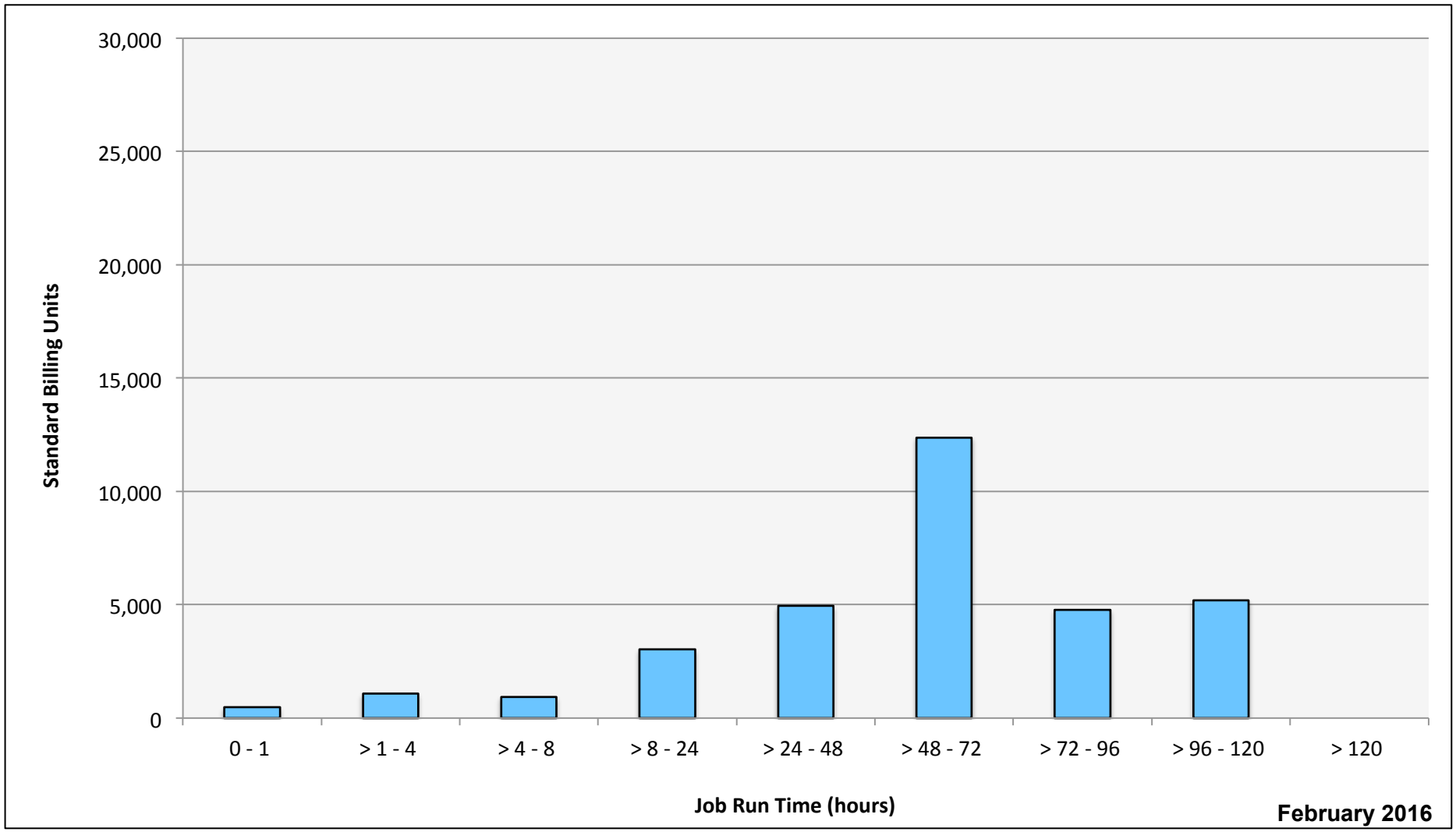
Merope:
Average Expansion Factor



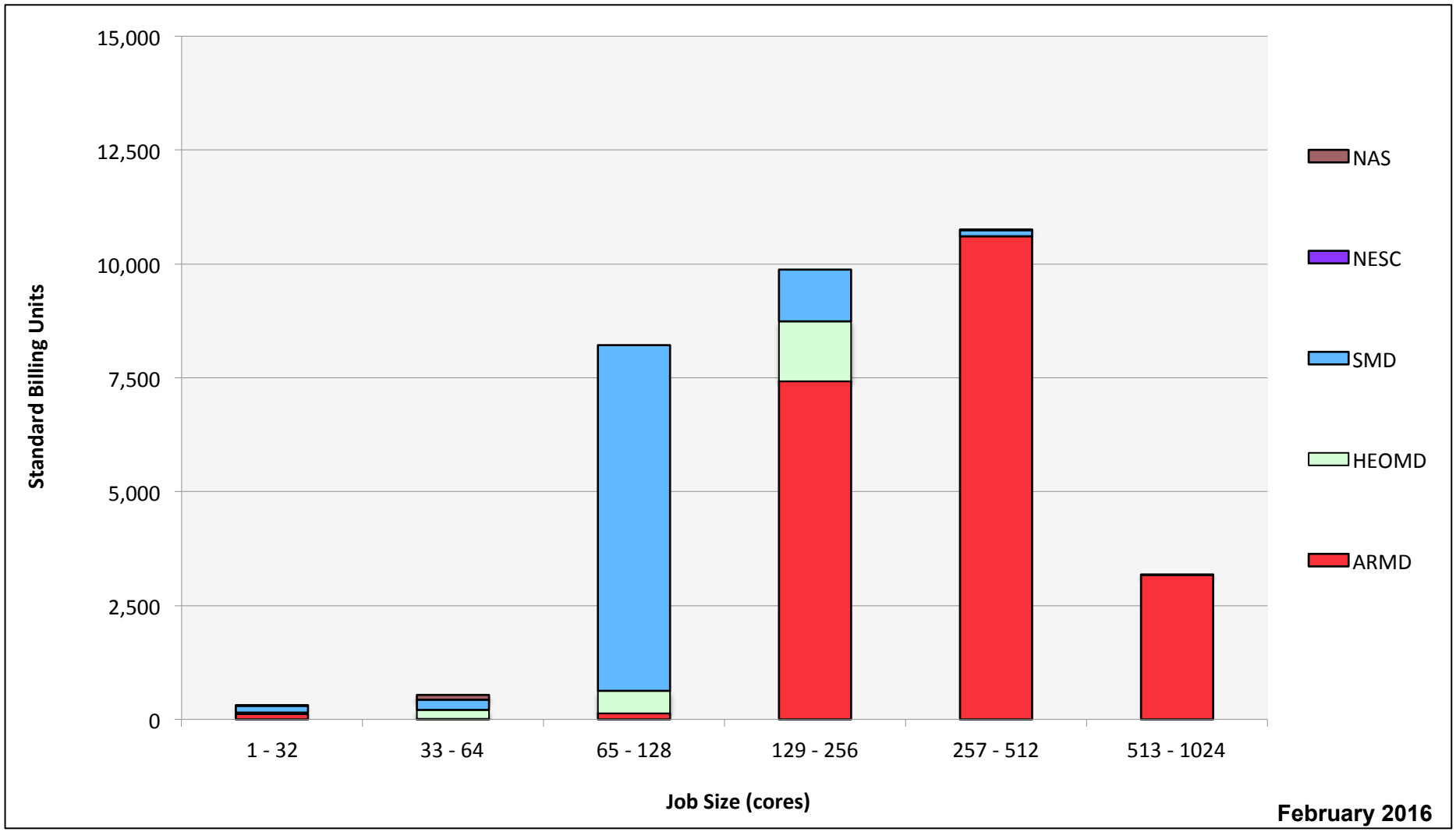
Endeavour:
SBUs Reported, Normalized to 30-Day Month



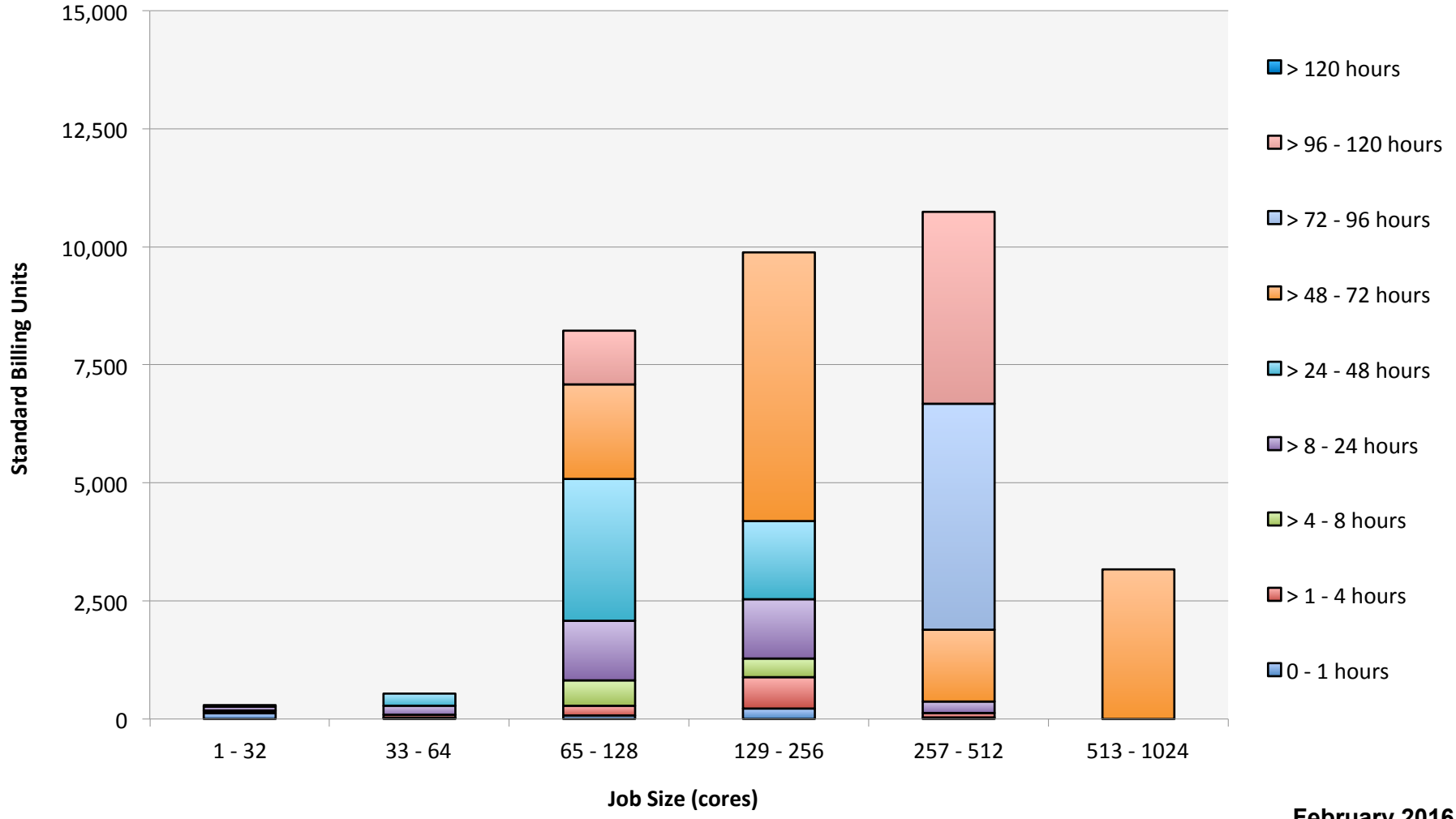
Endeavour:
Monthly Utilization by Job Length



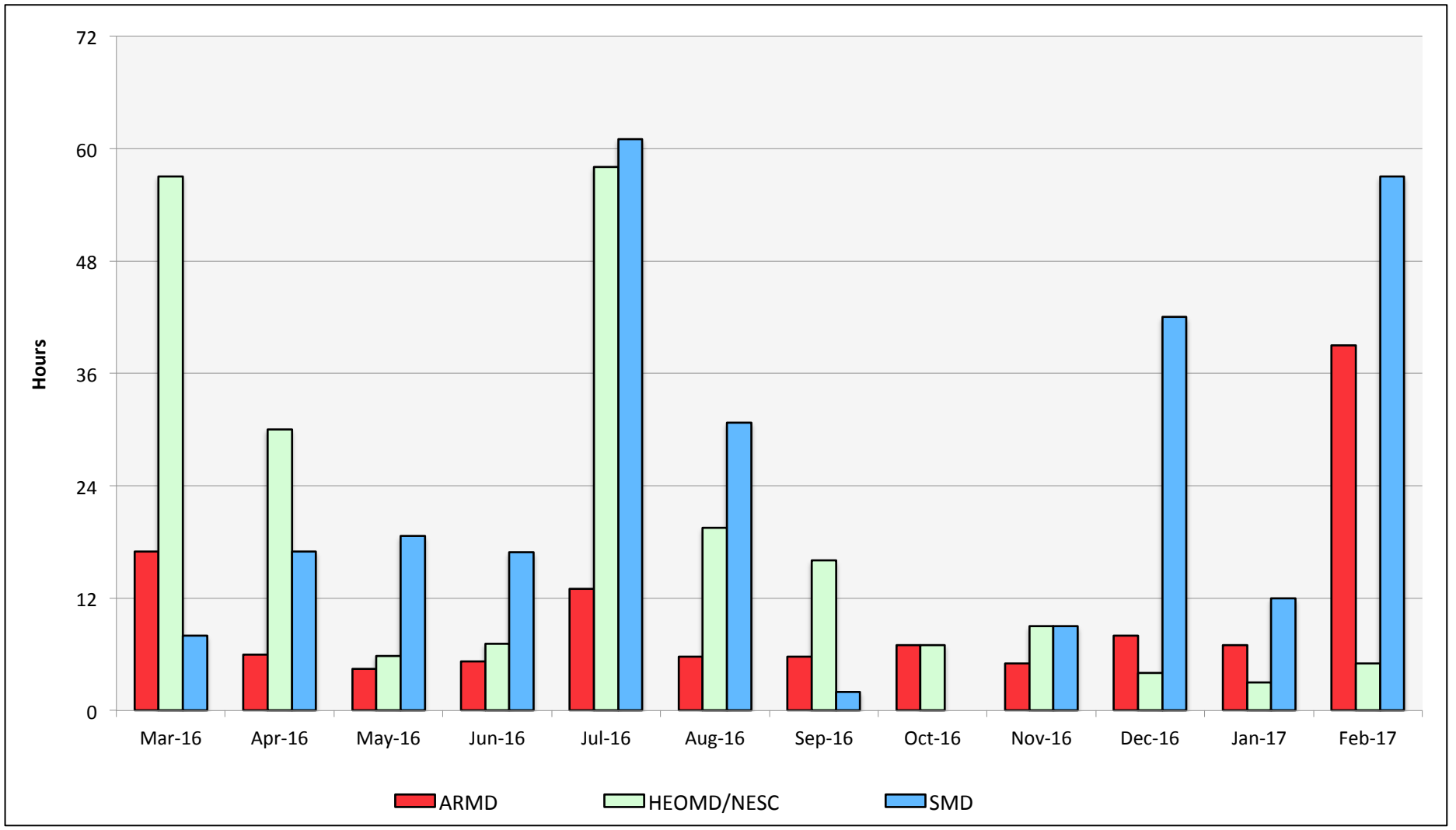
Endeavour:
Monthly Utilization by Size and Mission



Endeavour:
Monthly Utilization by Size and Length



Endeavour:
Average Time to Clear All Jobs



Endeavour:
Average Expansion Factor